

CAS SciFinder Discovery Platform™ (Academic)

AI 应用及最新进展



china@acs-i.org

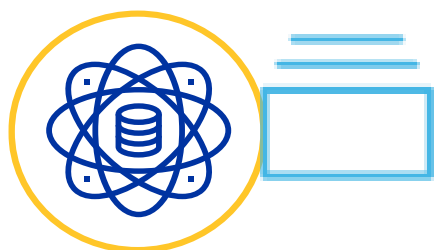
美国化学文摘社 (CAS) 北京代表处

大纲

- 美国化学文摘社（CAS）与 CAS SciFinder Discovery Platform 简介
- AI 应用助力快速发现目标研究信息
- CAS 加强对专利信息挖掘的支持
- 全面开放生命科学领域数据与表征信息

美国化学文摘社 (CAS) 隶属美国化学会 (ACS)

- 拥有超过 110 年的经验，创立权威化学索引《化学文摘》 (CA)
- 密切追踪、标引和提炼全球化学相关的文献 (包括专利)
- 提供各种科学信息和相关技术产品与服务
- 协助创新和保护创新，助力于解决科研方面的难题与挑战



UNPARALLELED
SCIENTIFIC CONTENT



SPECIALIZED
TECHNOLOGY



UNMATCHED
HUMAN EXPERTISE



CAS 数据覆盖学科

五大类 80 小类

—生物化学：

农化产品管控信息、生化遗传学、发酵、免疫化学、药理学

—有机化学各领域：

氨基酸、生物分子、碳水化合物、有机金属化合物、类固醇

—大分子化学各领域：

纤维素、木质素、造纸；涂料、墨水

染料、有机颜料；合成橡胶；纺织品、纤维

—应用化学各领域：

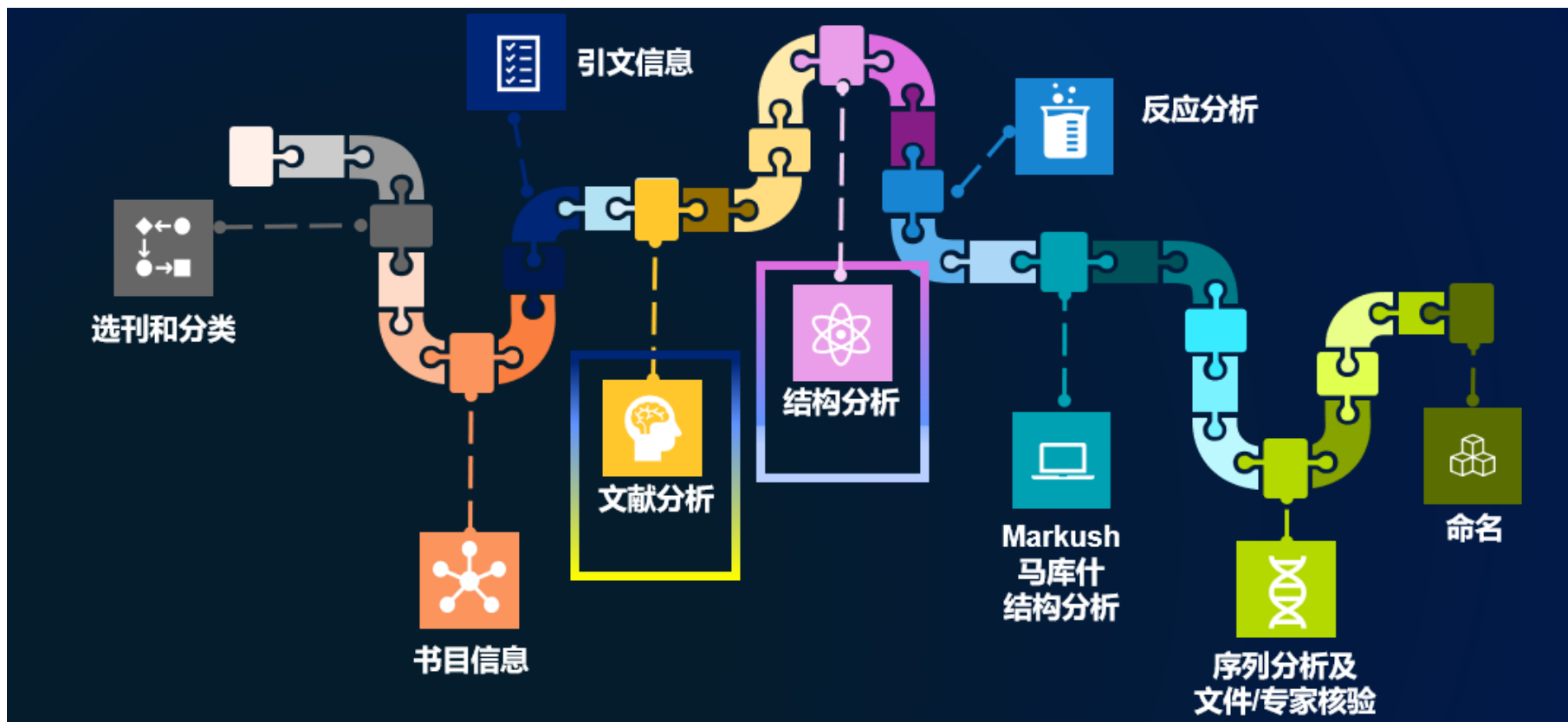
大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金

—物理、无机、分析化学各领域：

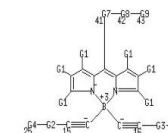
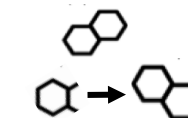
表面化学、催化剂、相平衡、核现象、电化学

CAS 科学家的智力标引

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



1990
Smith, M.
anthracene



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

经过 CAS 科学家的揭示，相关信息更易被挖掘

- 人工标引——精准揭示关键技术信息
- 科学家组成的编辑团队深刻理解客户的实际需求
- 审阅、筛选、摘要、标引以覆盖并揭示全球所有已公开的化学及相关信息
- CAS 登记号——物质的黄金标准
- CAS Roles (CAS 物质角色)——生物研究、性能用途、分析检测、合成制备
- CAS Index Terms (CAS 技术词语标准)——揭示技术词语相互间的关联
- CA Sections (CAS 学科分类, 80个类别)——精准定位具体研究领域

CAS 解决方案与服务



Discovery

CAS SciFinder Discovery Platform™

Get discoveries to market faster and optimize margins by giving researchers the information they need



Intellectual Property

STN IP Protection Suite™

Ensure that your intellectual property is protected and find opportunities to extend into new markets



Custom Solutions

CAS Custom ServicesSM

Customized data, analytics and insights to maximize the value of information assets and fuel digitalization success

CAS SciFinder Discovery Platform 平台解决方案

CAS SciFinderⁿ——加速科学发现的业界领先的科学工具

业界最领先的相关性搜索引擎，提供和化学相关的各学科文献、物质、反应和生物序列等检索内容，检索智能、高效、简单。可用于基金申请的文献准备、为新课题制定实验计划、寻求学术合作者、进行逆合成分析以及更多其他的教学和科研活动。

CAS Analytical Methods ——借助 CAS 科学家深度加工的科学方法，提升研究效率

分析方法解决方案涵盖来自期刊中的化学分析方法，提供检索和对比功能，可快速获得能直接在实验室操作的分析方法。可为法医学、食品科学、农学、制药、环境等学科的教学和实验提供帮助。

CAS Formulus ——助力开发安全、有效的产品

集成配方（制剂）数据与工作流程的解决方案，提供来自期刊、专利和产品说明中的配方详情。可检索制药、化妆品、食品、农化、油墨、涂料等众多领域中的配方，及其工艺、成分、目标成分的常见配伍成分、设计配方、和探索合规要求等。

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想借助代理 AI，直接获取关键问题的洞察信息？

EGFR有多少种突变？帮我详细列出已报道的突变类型，针对这些突变，有生物活性的小分子有哪些？

根据我在CAS SciFinder中的搜索结果，我为您整理了关于EGFR突变及其靶向小分子抑制剂的详细信息：

EGFR突变类型概述

CAS SciFinder中有 [188,352 references on EGFR mutations](#) 篇关于EGFR突变的文献。根据文献分析，EGFR突变可以分为以下几大类：

1. 常见敏感突变 (Classical/Sensitizing Mutations) - 占80-90%
 - Exon 19缺失 (最常见的是 delE746_A750)
 - Exon 21 L858R点突变
2. 不常见突变 (Uncommon Mutations) - 占10-20%
 - 2.1 敏感型不常见突变
 - Exon 18突变：
 - G719X (G719A/C/S)
 - E709A/V
 - Exon 18 indels
 - Exon 19突变：

How can I help you?

0/1000 characters

AI-generated content may contain inaccuracies. Please double-check cited sources. [Learn More](#)

依托 CAS 经过人工标引的公开科学数据提供简明见解，确保信息准确且科学严谨

你提到的第三代突变选择性抑制剂奥希替尼如何合成？

完美！现在我可以为您提供奥希替尼的详细合成路线信息：

奥希替尼 (Osimertinib) 的合成路线

根据CAS SciFinder数据库，奥希替尼有 456 synthetic routes to osimertinib 条合成路线。我为您详细介绍一条**六步合成路线**，该路线从商业化起始原料出发，总收率为**40.4%**。

合成路线总览

起始原料: 4-Fluoro-2-methoxyaniline (CAS 450-91-9)

最终产物: Osimertinib (CAS 1421373-65-0)

总步骤: 6步

总收率: 40.4%

详细合成步骤

步骤 1: 区域选择性硝化反应

How can I help you?

0/1000 characters

AI-generated content may contain inaccuracies. Please double-check cited sources. [Learn More](#)

支持多轮互动，可连贯上下文，提供跨研究领域的互联信息

CAS Newton是一款专为科学发现而打造的、具备科学智能的代理式人工智能。可有效降低获取可信科学知识的门槛，高效获取可靠分析与见解。

智能识别检索意图，助力快速获取研究信息

The screenshot displays the CAS SciFinder search interface. At the top left, the CAS SciFinder logo is visible. Below the logo, the text "Good Evening," is shown. A search bar contains the text "EGFR inhibitor". A dropdown menu is open, listing several search suggestions: "EGFR inhibitor", "EGFR inhibitors", "EGFR inhibitor SP101", "EGFR inhibitor PET1 peptide", "Tyrosine kinase EGFR inhibitor", "Receptor tyrosine kinase EGFR inhibitors", and a long text entry starting with "121-281-Cytokine TNFSF10 (tumor necrosis factor superfamily member 10) (human soluble isoform C-terminal fragment) fusion protein with Peptide (synthetic EGF in...". A yellow callout box with the text "智能检索框新增便捷自动建议功能" (Smart search box adds convenient automatic suggestion function) is overlaid on the first suggestion. At the bottom of the interface, there are two feature boxes: one with a DNA double helix icon and the text "Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.", and another with a document icon and the text "AI-enhanced prior art search for patent professionals."

AI 优化的文献检索，显著提升检索结果准确性

The screenshot displays the CAS SciFinder search results page for the query "siRNA side chain modification". The interface includes a search bar at the top with the query text, a navigation menu with options like "All", "Substances", "Reactions", "References", "Suppliers", and "Patent Markush", and a "Query Interpretation" panel on the right. The main results area shows 31 results, sorted by relevance, with a "View Related Results" dropdown. A prominent "AI Summary" box provides a key finding: "Based on the search results, here's a summary of key findings related to siRNA and side chain and modification: The search results highlight various studies focusing on the use of side chain modifications in polymers for siRNA delivery. Researchers have explored different approaches to enhance the efficiency and safety of siRNA delivery, including the introduction of hydrophobic side chains...". Below this, a list of document types is shown, with "Journal" being the most frequent. A specific article is highlighted: "Role of Hydrophobic Modification in Spermine-Based Poly(β -amino ester)s for siRNA Delivery and Their Spray-Dried Powders for Inhalation and Improved Storage". The article details authors (Jin, Yao; Wang, Xiaoxuan; Kromer, Adrian P. E.; Mueller, Joschka T.; Zimmermann, Christoph; Xu, Zehua; Hartschuh, Achim; Adams, Friederike; Merkel, Olivia M.) and publication information (Biomacromolecules (2024), 25(7), 4177-4191). A chemical structure diagram is also visible. The "Query Interpretation" panel on the right shows the interpretation of the search query as "siRNA and side chain and modification" and offers a "Search Original Query" button. A yellow callout box highlights the "Query Interpretation" panel and the "AI Summary" box, with the text: "可查看具体的AI检索解释，也可重新运行未经过 AI 增强的查询结果".

AI 赋能的检索结果总结，助力快速掌握关键发现

通过自然语言（如Info on, Information about等）便捷获取AI Summary结果

The screenshot displays a search interface for "Polyols from depolymerization of polyurethanes". The interface includes a search bar, navigation tabs (All, Substances, Reactions, References, Suppliers, Patent Markush), and a filter sidebar. The main content area shows a list of results, with the first result highlighted. A yellow box highlights the "View All" button for the AI Summary of the first result. A yellow arrow points from this button to a detailed AI Summary panel on the right. The AI Summary panel provides a concise overview of key findings and lists specific techniques and materials.

References search for "Polyols from depolymerization of polyurethanes"

Query Interpretation ⓘ

🔍 All 📦 Substances ⚗️ Reactions 📄 References 🛒 Suppliers 📄 Patent Markush

View Related Results ▾

Filter Results <

Analyze Results

Behavior

Filter by Exclude

Search Within Results

Search for up to 3 text strings within the result set.

Enter a query...

Search

Document Type

Journal (167)

Patent (174)

Review (16)

Conference (10)

Flags

347 Results Sort: Relevance ▾ View: Partial Abstract ▾

AI Summary

Based on the search results, here's a summary of key findings related to polyols and depolymerization and polyurethanes:

The search results highlight various methods for the depolymerization of polyurethanes to produce polyols, which can be used in the production of new polyurethane materials. Hydrolysis, glycolysis, and acidolysis are among the techniques used for the depolymerization of polyurethanes, with the aim of creating bio-based polyols from waste materials. These methods can be applied to different types of polyurethanes, including rigid and flexible foams, and can achieve high recovery rates of polyols. Additionally, the use of lignin as a source of bio-based polyols is explored, with depolymerization of lignin to produce polyols for rigid polyurethane foam production. The recovered polyols can be used in the formulation of new polyurethane materials, demonstrating the potential for closed-loop recycling of polyurethanes.

View All ▾

1

Depolymerization of lignins and their applications for the preparation of polyols and rigid polyurethane foams: A review

By: Mahmood, Nubla; Yuan, Zhongshun; Schmidt, John; Xu, Chunbao
Renewable & Sustainable Energy Reviews (2016), 60, 317-329 | Language: English, Database: CAplus

A review. Lignin, nature's dominant aromatic polymer, is found in most terrestrial plants in the range of 15-40% dry weight and provides structural integrity. Kraft lignin (KL) is a major byproduct of pulp & paper industry where, hydrolysis lignin (HL) is the solid residue left from the enzymic hydrolysis of wood after the pretreatment processes in cellulosic ethanol plants. Currently, most of the lignin is burned to generate heat and electricity and remaining is considered as a low value material. Only 1% of the annually produced lignin is being commercialized for its application in the p...

AI Summary

Based on the search results, here's a summary of key findings related to polyols and depolymerization and polyurethanes:

The search results highlight various methods for the depolymerization of polyurethanes to produce polyols, which can be used in the production of new polyurethane materials. Hydrolysis, glycolysis, and acidolysis are among the techniques used for the depolymerization of polyurethanes, with the aim of creating bio-based polyols from waste materials. These methods can be applied to different types of polyurethanes, including rigid and flexible foams, and can achieve high recovery rates of polyols. Additionally, the use of lignin as a source of bio-based polyols is explored, with depolymerization of lignin to produce polyols for rigid polyurethane foam production. The recovered polyols can be used in the formulation of new polyurethane materials, demonstrating the potential for closed-loop recycling of polyurethanes.

Key Findings:

- Depolymerization Techniques:**
 - Hydrolysis, glycolysis, and acidolysis are effective methods for depolymerizing polyurethanes to produce polyols. (2) (7)
 - Multi-stage degradation (MSD) method can efficiently degrade polyurethane materials to recover polymerizable polyols. (8)
- Bio-Based Polyols:**
 - Lignin can be depolymerized to produce bio-based polyols for rigid polyurethane foam production. (1) (12)
 - Corn cob lignin can be depolymerized into bio-polyols with low molecular weight and suitable hydroxyl number for rigid polyurethane foam synthesis. (12)
- Waste Utilization:**

基于相关性排序，获取前20个文献结果的总结，既提供宏观概览，也包含更详细的信息

支持自然语言直接检索物质理化性质，直观高效

Results for "what is the boiling point of DMF"

All Substances Reactions References Suppliers Patent Markush

68-12-2
DMF

Boiling Point
153 °C
Condition Press: 760 Torr
Source
"Hazardous Substances Data Bank" data were obtained from the National Library of Medicine (US)

Boiling Point Properties
Showing 5 of 210 Results [View in Detail Page →](#)

Value	Condition	Source
153 °C	Press: 760 Torr	"Hazardous Substances Data Bank" data were obtained from the ...

Results for "the logP of olaparib"

All Substances Reactions References Suppliers Patent Markush

763113-22-0
Olaparib

logP
1.037±0.00
Condition Temp: 25 °C
Source

logP Properties
Showing 1 of 1 Result [View in Detail Page →](#)

Value	Condition	Source
1.037±0.00	Temp: 25 °C	Calculated using Advanced Chemistry Development (ACD/Labs) S...

无需多次点击，
直接展示目标属性

CAS 标引的参数
均支持自然语言
检索

Experimental Properties

Acoustic	Biological	Chemical	Density	Electrical	Flow and Diffusion	Interface	Lipinski	Magnetic	Mechanical	Optical and Scattering	Thermal
Property	Value	Condition	Source								
Sound Velocity	1541.09 m/s (liquid)	Temp: 298 K; Press: 1.01325 x 10 ⁵ Pa; λ: 2 MHz	(1) CAS								
Sound Velocity	1497.70 m/s (liquid)	Temp: 298 K; Press: 1.01325 x 10 ⁵ Pa; λ: 2 MHz	(1) CAS								
Sound Velocity	1477.8 m/s (approx)	Temp: 293 K; Press: 1 x 10 ⁵ Pa	(2) CAS								

扩展问答类型，自然语言快速聚焦物质谱图

Results for "the proton spectra of ibuprofen"

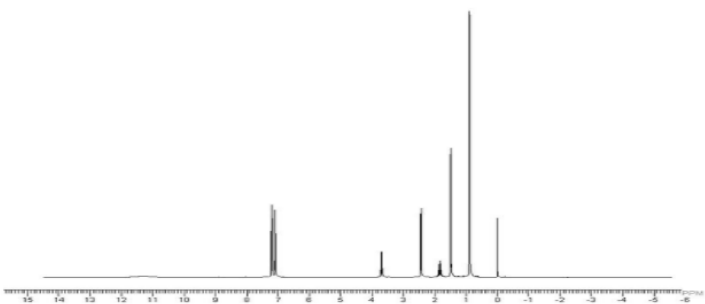
All Substances Reactions References Suppliers Patent Markush

Spectra **无需多次点击和跳转，核磁谱图即查即得** View All Spectra →

Showing 5 of 28 Results

15687-27-1
Ibuprofen
Viewing 1 of 5

Experimental
View Spectra Details



Proton NMR Spectrum

Conditions

Working Frequency
300 MHz

Solvent
Chloroform-d (865-49-6)

Spectra Summary

Spectrum ID
SLSH_005579

Source
Sigma-Aldrich Co. LLC. (Spectr...)

View All ↓

Experimental Spectra							
<u>¹H NMR</u>	¹³ C NMR	IR	Mass	Raman	UV and Visible	X-Ray	Additional Spectra
View Proton NMR Spectrum (Image Available)						Solvent	Source
View Proton NMR Spectrum (Image Available)						Chloroform-d	(1) WSA
View Proton NMR Spectrum (Image Available)						DMSO-d ₆	(2) ENAMINE

自然语言检索反应有效降低检索难度

Reactions search for "synthesis of aliphatic aldehydes from alcohols"

☰ All ☑ Substances **☑ Reactions** 📄 References 🛒 Suppliers 📄 Patent Markush

View Related Results ▾

Filter Results <

Behavior

Filter by Exclude

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

Reagent

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

18,086 Results

1

Oxidation or Dehydrogenation of Alcohols to Aldehydes and Ketones

View 11661 Related Reactions

R-CH(OH)-R1

2

Oxidation of Primary Alcohols to Carboxylic Acids or Carboxylic Anhydrides

View 1242 Related Reactions

R-CH2-OH

Reactions search for "synthesis from Trastuzumab"

☰ All ☑ Substances **☑ Reactions** 📄 References 🛒 Suppliers 📄 Patent Markush

View Related Results ▾

Filter Results <

Behavior

Filter by Exclude

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

Reagent

Yield

90-100% (39)

80-89% (1)

70-79% (1)

50-69% (7)

210 Results

Group: By Scheme ▾ Sort: Publication Date: Newest ▾ View: Collapsed ▾

Scheme 1 (1 Reaction) Steps: 1 Yield: 90% ***

180288-69-1 Image Not Available + 3066517-86-7 Image Not Available

Suppliers (28)

conjugates with Herceptin

Expand Scheme ▾

Scheme 2 (1 Reaction) Steps: 1 Yield: 90% ***

180288-69-1 Image Not Available + 3066518-00-8 Image Not Available

Suppliers (28)

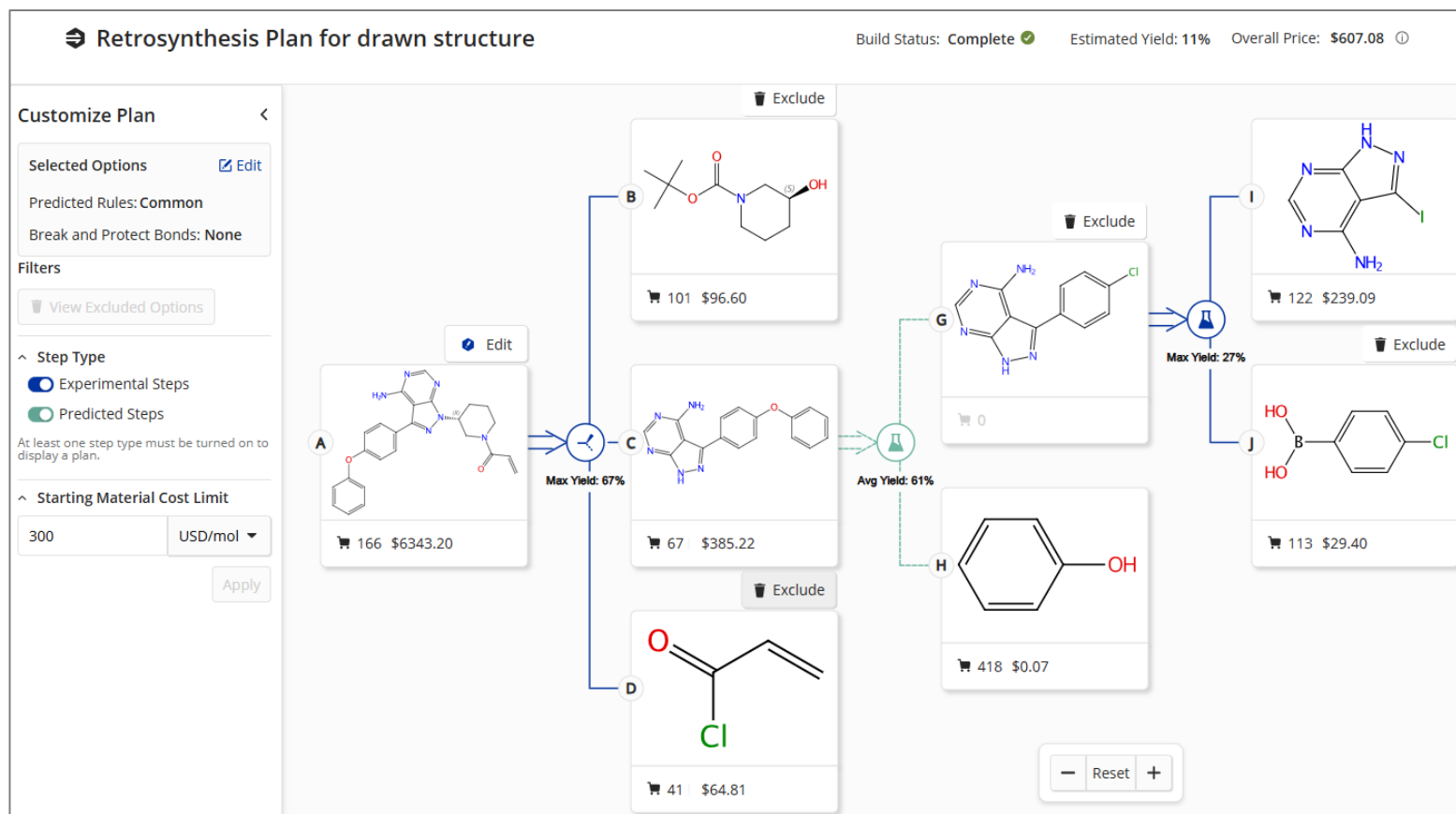
conjugates with Herceptin

Expand Scheme ▾

检索一类反应担心结构式绘制不全面？
检索关键官能团，在结果中浏览转化类型

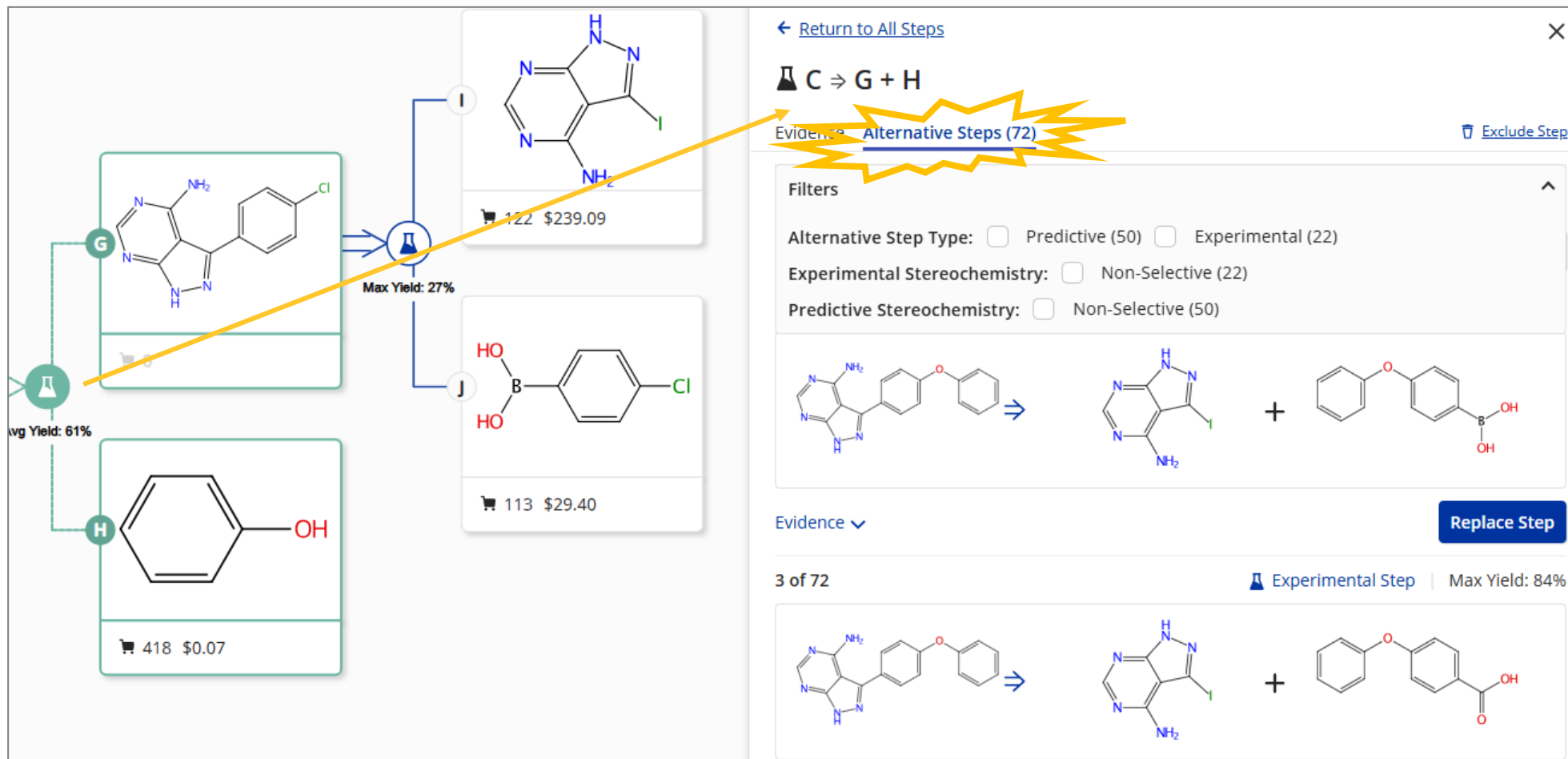
结构式太复杂绘制不方便？
物质名直接检索反应，快速获取目标结果

逆合成路线用时大幅减少，AI 和数据驱动高效研发



- 无需等待，快速获得逆合成路线，“即查即得”
- 拓宽设计思路，AI 支持的预测路线让路线优化更简单全面
- 助力评估合成难度，为立项和早期筛选提供决策依据

逆合成路线用时大幅减少，AI 和数据驱动高效研发



不止一条反应路线，每步反应均提供丰富的替换路线

重点回顾

AI 应用助力快速发现目标研究信息

上线代理 AI 工具 CAS Newton，降低获取可信数据门槛，高效查阅可靠分析与见解；智能识别检索意图，可利用自然语言检索物质属性、反应信息和文献，信息检索更直观高效；借助 AI 技术与 CAS 标引的高质量数据，优化逆合成路线设计

大纲

- 美国化学文摘社（CAS）与 CAS SciFinder Discovery Platform 简介
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结构编辑器可直接指定检索类型，提升检索效率

The screenshot displays the CAS Draw software interface. At the top, a dropdown menu is set to "CAS Draw". Below it, a "Select Search Type" section contains several tabs: "Substances", "References", "Reactions", "Suppliers", "Patent Markush", and "All". The "References" tab is highlighted with a blue background and a yellow border. The main workspace shows a chemical structure of a complex molecule consisting of a benzene ring connected to a pyridine ring, which is further connected to a quinoline ring system with two oxygen atoms. A tooltip box is overlaid on the right side of the workspace, containing the following text:

Enter a single IUPAC Name, CAS Registry Number, SMILES string or InChI, then press [Enter] or click on the Add to Editor icon.

Examples:

1,2-Dibromoethane
50-78-2
CC(=O)Oc1ccccc1C(=O)O
InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)

At the bottom of the interface, the molecular formula is displayed as C15H13N3O2 (267.29). A search bar at the bottom left contains the letter "N". A zoom slider at the bottom center is set to 100%. "Cancel" and "OK" buttons are located at the bottom right.

Prior Art Discovery 便捷获取现有技术信息

基于AI技术和CAS科学家标引内容，助力可专利性和专利风险评估

Prior Art Discovery
Discover prior art in patents and non-patent literature using AI-enhanced search technologies.

✦ Prior Art Discovery

基于指定信息的现有技术探索

Prior Art Discovery uses CAS AI tools to find similar patents and non-patent literature results. [Learn more about Prior Art Discovery.](#)

This disclosure is related to the field of processes to produce molecules that are useful as pesticides (e.g., acaricides, insecticides, molluscicides, and nematocides), such molecules, and processes of using such molecules to control pests. In general, the molecules of Formula One may be used to control pests e.g. beetles, earwigs, cockroaches, flies, aphids, scales, whiteflies, leafhoppers, ants, wasps, termites, moths, butterflies, lice, grasshoppers, locusts, crickets, fleas, thrips, bristletails, mites, ticks, nematodes, and symphylans. Generally, when the molecules disclosed in Formula One are used in a formulation, such formulation can also contain other components. These components include, but are not limited to, (this is a non-exhaustive and non-mutually exclusive list) wetters, spreaders, stickers, penetrants, buffers, sequestering agents, drift reduction agents, compatibility agents, anti-foam agents, cleaning agents, and emulsifiers.

输入不少于200个英文字符的自然语言，进行现有技术探索

Priority Date: 08-12-2025 [Edit](#)

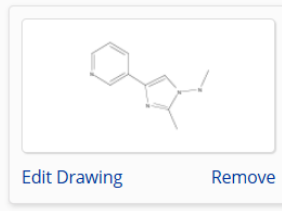
自定义优先权日期

962 / 10,000 characters [Clear Text](#)

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Search



可添加结构

Prior Art Discovery 直观呈现相关的现有技术报道

✦ Prior Art Discovery for "This disclosure is related to the field of processes to produce molecules that are useful as pesticides (e..."

Search Details

Your Inputs

Text

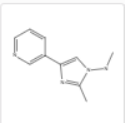
This disclosure is related to the field of processes to produce molecules that are usefu...

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Priority Date

08-12-2025

Structure



Patents (100) Non-Patent Literature (83)

Sort: Relevance

1

Pyridinylimidazoles as pesticidal and processes for preparation and pesticidal composition

Assignee: Dow AgroSciences LLC
US20120110701 A1, Publication Date: 2012-05-03 | Priority Date: 2010-11-03

...to pyridinylimidazoles of **formula I** as **pesticides** useful in pest control. Compounds of **formula I** wherein X is N and XR8; R1, R2, R3, R4 and R8 are independently H, F, Cl, Br, I, CN, etc.; R5 is H, (un)substituted C1-6...

Full Text

2

Preparation of substituted 4-(3-phenylbut-1-en-1-yl)benzoylhydrazinecarboxamides as pesticides

Assignee: Dow AgroSciences LLC
US20170208810 A1, Publication Date: 2017-07-27 | Priority Date: 2016-01-25

...amidating (Z)-2-bromo-4-(1,4,4,4-tetrafluoro-3-(3,4,5-trichlorophenyl)but-1-en-1-yl)benzoic acid (preparation given) with N-(2,2,2-trifluoroethyl)hydrazinecarboxamide hydrochloride afforded 13% (Z)-II. Exemplified compounds I were tested for their pesticidal activity (data given for representative compounds I). Compounds I and compositions may be used, for example, as acaricides, **insecticides**, miticides, **molluscicides**, and **nematicides**.

Full Text

3

Pyridinylimidazoles as pesticidal and processes for preparation and pesticidal composition

Assignee: Dow AgroSciences LLC
US20120110701 A1, Publication Date: 2012-05-03 | Priority Date: 2010-11-03

...to pyridinylimidazoles of **formula I** as **pesticides** useful in pest control. Compounds of **formula I** wherein X is N and XR8; R1, R2, R3, R4 and R8 are independently H, F, Cl, Br, I, CN, etc.; R5 is H, (un)substituted C1-6...

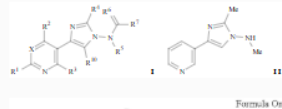
Pyridinylimidazoles as pesticidal and processes for preparation and pesticidal composition

Assignee: Dow AgroSciences LLC

Patent

View Reference Details

The invention relates to pyridinylimidazoles of **formula I** as **pesticides** useful in pest control. Compounds of **formula I** wherein X is N and XR8; R1, R2, R3, R4 and R8 are independently H, F, Cl, Br, I, CN, etc.; R5 is H, (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl, (un)substituted C2-6 alkynyl, etc.; R6 is O, S, NH and derivatives, NOH and derivatives; R7 is (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl, (un)substituted C1-6 alkoxy, etc.; are claimed. Example compound II was prepared by condensation of tert-Bu 1-methylhydrazinecarboxylate with Et acetimidate hydrochloride; the resulting N'-(1-iminoethyl)-N-methylhydrazinecarboxylic acid tert-Bu ester underwent heterocyclization with 2-bromo-1-(pyridin-3-yl)ethanone hydrochloride to give Me (2-methyl-4-pyridin-3-ylimidazol-1-yl)carbamic acid tert-Bu ester, which underwent hydrolysis to give compound II. All the invention compounds were evaluated for their pesticidal activity (some data given).



Publication Information View More

Hit Structures

1374355-36-8



N,2-Dimethyl-4-(3-pyridinyl)-1H-imidazol-1-amine

Concepts

- Acari
- Agrochemical formulations
- Agrochemical microcapsules
- Allopaupropus
- Animals
- Anoplura
- Antibacterial agents
- Antiviral agents
- Aphidoidea
- Arachnida

View All

Claims

Claims text may be based on automatic Optical Character Recognition processes.

1. What is claimed is:

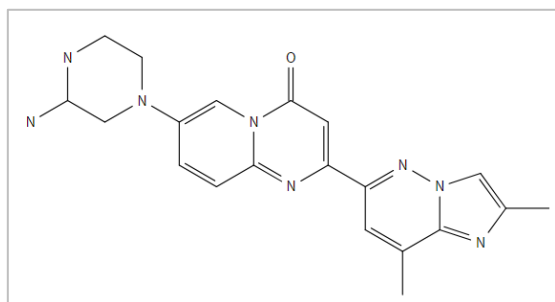
A composition comprising a **molecule** according to **Formula One**:

View All

CAS Markush 检索助力快速进行可专利性评估

CAS Markush 数据集是专利审查员重要的参考依据

Patent Markush
Search Patent Markush by structure and view associated references.



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Patent Markush search for drawn structure

All Substances Reactions References Suppliers Patent Markush

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Patent Markush Match

As Drawn (1)

Substructure (1)

Behavior

Filter by Exclude

Patent Office

World Intellectual Property Organization (1)

CA Section

1 Result

1

深入Markush结构详情

WO2017081111 Markush Details

Preparation of substituted 2-(imidazo[1,2-b]pyridazin-6-yl)-pyrido[1,2-a]pyrimidin-4-ones for treating amyotrophic lateral sclerosis

Assignees: F. Hoffmann-La Roche AG; Hoffmann-La Roche Inc.
World Intellectual Property Organization, WO2017081111 A1 2017-05-18 | Language: English, Database: CAPlus

Patent Status: Dead

Patent claim 1

PatentPak Full Text

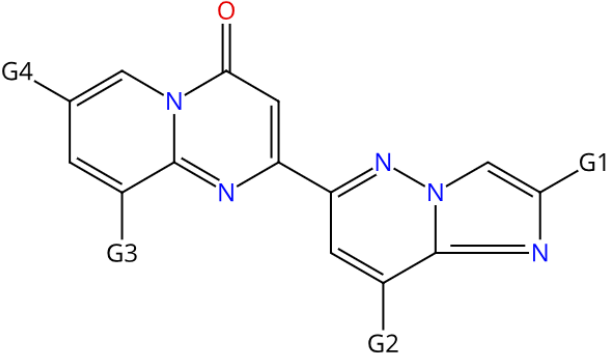
453,454,455,456,457: opt. substd. by G22

629: opt. substd.

CAS 科学家拆解与解读的 Markush 结构详情

Patent Markush 1

PatentPak Full Text

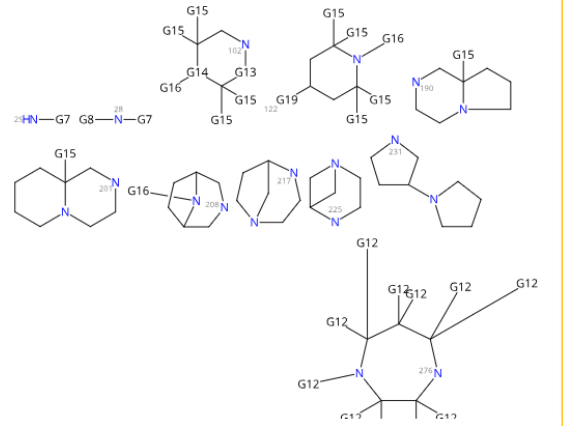


Reset

Publication Information
 Assignees: F. Hoffmann-La Roche AG; Hoffmann-La Roche Inc.
 World Intellectual Property Organization, WO2017081111 A1 2017-05-18 | Language: English, Database: CAplus

Notes
 Patent claim 1
 or pharmaceutically acceptable salts
 substitution is restricted
 additional ring formation also claimed

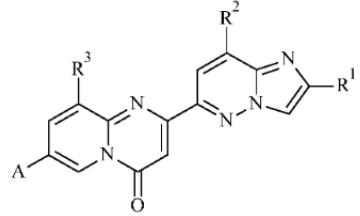
G1 = H \ alkyl \ Me
 G2 = H \ CN \ alkyl (opt. substd. by G5) \ cycloalkyl \ Me
 G3 = H \ alkyl \ cycloalkyl \ Me
 G4 = heterocycle (opt. substd. by G6) \ 25 \ 28 \ 102 \ 122 \ 190 \ 201 \ 208 \ 217 \ 225 \ 231 \ 245 \ 250 \ piperazino (opt. substd. by G22) \ 276 \ 355 \ 374 \ pyrrolidino (opt. substd. by G22) \ 299 \ 318 \ 330 \ 339 \ 349



清晰直观展示原文中复杂 Markush 结构的拆解与解读，助力快速进行FTO分析

Claims

1. The compound of formula (I)



(I)

wherein

5 R¹ is hydrogen or C₁₋₇-alkyl;
 R² is hydrogen, cyano, C₁₋₇-alkyl, C₁₋₇-haloalkyl or C₃₋₈-cycloalkyl;
 R³ is hydrogen, C₁₋₇-alkyl, or C₃₋₈-cycloalkyl;
 A is N-heterocycloalkyl or NR¹²R¹³, wherein N-heterocycloalkyl comprises 1 or 2 nitrogen ring atoms and is optionally substituted with 1, 2, 3 or 4 substituents selected from R¹⁴;

10 R¹² is heterocycloalkyl comprising 1 nitrogen ring atom, wherein heterocycloalkyl is optionally substituted with 1, 2, 3 or 4 substituents selected from R¹⁴;
 R¹³ is hydrogen, C₁₋₇-alkyl or C₃₋₈-cycloalkyl;

原文 Markush 结构

CAS 科学家对文献多维度标引，快速获取研究重点

Preparation of EGFR inhibitor-E3 ubiquitin ligase ligand conjugates as targeted degraders for treatment of cancer

330 957 2 Citation Map

专利详情页显示专利权人信息

Assignee: BeiGene, Ltd.
Inventors: Lei, Bailin; Liu, Huaqing; Han, Songzhe; Wang, Zhiwei

Disclosed herein are novel bifunctional compounds of formula I formed by conjugating EGFR inhibitor moieties with E3 ligase Ligand moieties, which function to recruit targeted proteins to E3 ubiquitin ligase for degradation, and methods of preparation and uses thereof. Compounds of formula I [wherein R¹ = P(O)R^{1a}R^{1b}, SO₂R^{1a}, SO₂NR^{1a}R^{1b}, etc.; R^{1a} and R^{1b} each independently = H, C₁₋₈alkyl, C₃₋₈cycloalkyl, each optionally substituted with at least one halo; each Z⁵-Z⁸ independently = CR' or N, with at least one of Z⁵-Z⁸ = N; each R' independently = H, halo, C₁₋₈alkyl, C₃₋₈cycloalkyl, etc.; each Z¹-Z⁴ independently = CH, C-halo, N, etc.; R⁴ = H, halo, C₆₋₁₂aryl, etc.; L¹, L², and L³ independently = single bond, O, SO₂, CO, etc.; m₁ = 0 or 1; m₂ and m₃ independently = 0, 1, 2, 3, 4, 5, 6, 7, or 8; n = 0, 1, 2, or 3; degron = (2,6-dioxopiperidin-3-yl)-1-oxoisindolinyl, (2,6-dioxopiperidin-3-yl)-1H-indazolyl, (2,6-dioxopiperidin-3-yl)-2,6-difluorophenyl, etc.; X¹ and X² independently = CH, C-halo, N, etc.] or N-oxides, pharmaceutically acceptable salts, stereoisomers, or deuterated analogs thereof, are claimed and exemplified. Example compound II was prepared via a 5 step synthesis (preparation given)

导航速览

- Claims
- Classifications
- CAS Concepts
- Markush Structures
- Substances
- Reactions
- Pharmacological Data

专利分类代码中新增CPC代码

Patent	Classification	Codes
WO2022171123 A1	IPCI	A61K 31/506; C07D 401/12; A61P 35/00
CN116847848 A	IPCI	A61K 31/506
	CPCI	A61P 35/00; C07D 401/14; C07D 471/04; C07D 513/04; C07D 498/04; C07D 413/14; C07D 417/14; C07F 9/65583; C07F 9/6561; C07D 487/10
EP4291193 A1	IPCI	A61K 31/506; C07D 401/12; A61P 35/00
	CPCI	A61P 35/00; C07D 401/14; C07D 471/04; C07D 513/04; C07D 498/04; C07D 413/14; C07D 417/14; C07F 9/65583; C07F 9/6561; C07D 487/10
US20240165243 A1	IPCI	A61K 47/55; A61K 47/54
	CPCI	A61K 47/55; A61K 47/545

CAS 科学家对文献多维度标引，快速获取研究重点

增强的专利家族详情助力便捷查看同族专利信息

可筛选、排序的专利家族详情表，提升查看效率

Patent	Language	Full Text	Publication Date	Application Number	Application Date	Patent Status	Status Date
WO2016149668 A1	English	PatentPak PDF	2016-09-22	WO2016-US23258	2016-03-18	Dead	
CA2979070 A1	English	PatentPak PDF	2016-09-22	CA2016-2979070	2016-03-18	Alive	
US20160272639 A1	English	PatentPak PDF	2016-09-22	US2016-15074820	2016-03-18	Alive	
AU2016232705 A1	English	PatentPak PDF	2017-09-21	AU2016-232705	2016-03-18	Alive	
	English		2018-01-24	EP2016-765865	2016-03-18	Dead	
	Korean	PatentPak PDF	2018-02-02	KR2017-7030057	2016-03-18	Alive	
	Japanese	PatentPak PDF	2018-05-17	JP2018-500278	2016-03-18	Alive	2020-11-21
MX2017011919 A	Spanish		2018-05-22	MX2017-11919	2016-03-18	Alive	2025-04-10
BR112017019751 A2	Portuguese		2018-05-29	BR2017-112017019751	2016-03-18	Alive	2020-11-20
CN108601764 A	Chinese	PatentPak PDF	2018-09-28	CN2016-80022417	2016-03-18	Alive	2020-11-21
US10730870 B2	English	PatentPak PDF	2020-08-04	US2016-15074820	2016-03-18	Alive	2020-11-21
AU2016232705 B2	English	PatentPak PDF	2020-08-04	US2016-15074820	2016-03-18	Alive	2020-11-21
RU2782063 C2	Russian		2020-08-04	RU2016-15074820	2016-03-18	Alive	2020-11-21
JP7269731 B2	Japanese	PatentPak PDF	2020-08-04	JP2016-15074820	2016-03-18	Alive	2020-11-21
KR2616762 B1	Korean	PatentPak PDF	2020-08-04	KR2016-15074820	2016-03-18	Alive	2020-11-21
KR2023175343 A	Korean	PatentPak PDF	2020-08-04	KR2016-15074820	2016-03-18	Alive	2020-11-21
EP4414369 A2	English	PatentPak PDF	2020-08-04	EP2016-15074820	2016-03-18	Alive	2020-11-21
EP4414369 A3	English	PatentPak PDF	2020-08-04	EP2016-15074820	2016-03-18	Alive	2020-11-21
MX2021010482 A	Spanish		2020-08-04	MX2016-15074820	2016-03-18	Alive	2020-11-21
IN201737033221 A	English		2020-08-04	IN2016-15074820	2016-03-18	Alive	2020-11-21

合并的专利号与专利文献代码

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Filter Patent Status

- Alive (30)
- Dead (3)
- Unknown (1)

Clear Apply

CAS PatentPak

PAGE 232 / 244

ZOOM

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Key Substances in Patent

- CAS RN 9004-02-8 Lipoprotein lipase
- Analyst Markup Locations (1) Page 120
- CAS RN 9025-15-4

13. The compound of any of claims 1-12, wherein said polyethylene glycol group contains between 2 and 10 ethylene glycol units.

14. The compound of any of claims 1-13, wherein said PTM group is a moiety which binds to a target protein, wherein said target protein is selected from the group consisting of structural proteins, receptors, enzymes, cell surface proteins, proteins prominent to the integrated function of a cell, including proteins involved in catalytic activity, aromatase activity, motor activity, helicase activity, metabolic processes (anabolism and catabolism), antioxidant activity, proteolysis, glycosynthesis, proteins with kinase activity, oxidoreductase activity, transferase activity, hydrolase activity, lyase activity, isomerase activity, ligase activity, enzyme regulator activity, signal transducer activity, structural molecule activity, binding activity (protein, lipid carbohydrate), receptor activity, cell motility, membrane fusion, cell communication, regulation of biological processes, development, cell differentiation, response to stimulus,

CAS 科学家对文献多维度标引，快速获取研究重点

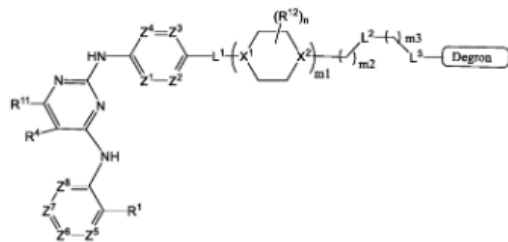
快速获取Claims与专利Markush信息，提升FTO效率

Claims

直接获取权利要求信息

Claims text may be based on automatic Optical Character Recognition processes.

- 1 What is claimed is:
A compound of Formula (X) :



(X)

or a N-oxide thereof, or a pharmaceutically acceptable salt thereof, or a stereoisomer thereof, or a deuterated analog
R¹ is selected from -P(O)R^{1a}R^{1b}, -SO₂R^{1a}, -SO₂NR^{1a}R^{1b} or -N(R^{1a})-SO₂R^{1b}, wherein R^{1a} and R^{1b} are each indep
said -C₁₋₈alkyl or C₃₋₈cycloalkyl is optionally substituted with at least one halogen;

Z⁵ is selected from -CR², or N;

Z⁶ is selected from -CR³, or N;

Z⁷ is selected from -CR⁹, or N;

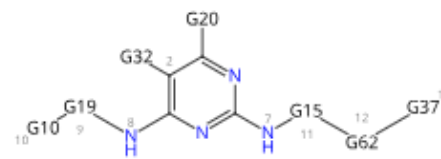
Z⁸ is selected from -CR¹⁰, or N;

at least one of Z⁵, Z⁶, Z⁷ and Z⁸ is N;

R² and R³ are each independently selected from hydrogen, halogen, -C₁₋₈alkyl, -C₂₋₈alkenyl, -C₂₋₈alkynyl, C₃₋₈cycloalkyl, 3-to 8-memb
membered heteroaryl, -CN, -OR^{2a}, -SO₂R^{2a}, -SO₂NR^{2a}R^{2b}, -COR^{2a}, -CO₂R^{2a}, -CONR^{2a}R^{2b}, -NR^{2a}R^{2b}, -NR^{2a}COR^{2b}, -NR^{2a}CO₂R^{2b}, or
-C₂₋₈alkenyl, -C₂₋₈alkynyl, C₃₋₈cycloalkyl, 3-to 8-membered heterocycl, C₆₋₁₂aryl or 5-to 12-membered heteroaryl is optionally substi
and R³ together with the carbon atoms to which they are attached, form a 5-6 membered saturated or partially or completely unsatur
aromatic) ring, said ring comprising 0-3 heteroatoms independently selected from nitrogen, oxygen or sulfur; said ring is optionally subs
R^{2e}, at each occurrence, is independently hydrogen, halogen, -C₁₋₈alkyl, -C₂₋₈alkenyl, -C₂₋₈alkynyl, -C₁₋₈alkoxy, -C₃₋₈cycloalkyl, oxo, 3-t
12-membered heteroaryl, -CN, -SO₂R^{2a}, -SO₂NR^{2a}R^{2b}, -COR^{2a}, -CO₂R^{2a}, -CONR^{2a}R^{2b}, -NR^{2a}R^{2b}, -NR^{2a}COR^{2b}, -NR^{2a}CO₂R^{2b} or -NR²

Markush Structures

Patent Markush 1



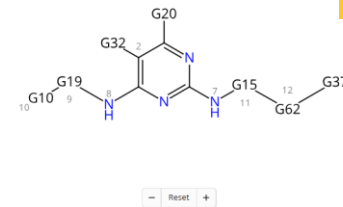
Notes

Patent claim 1

additional derivatization also claimed

[View all on Markush Detail](#)

清晰直观展示专利中复杂的Markush结构和定位

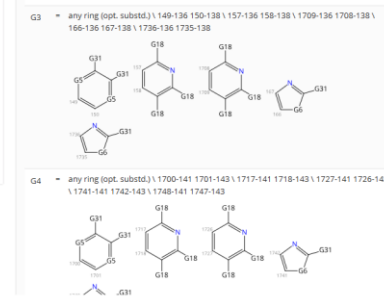


Publication Information

Assignee: BeiGene, Ltd.
World Intellectual Property Organization, WO202217123 A1 2022-06-18 | Language: English, Database: Caplus

Notes

Patent claim 1
additional derivatization also claimed
or N-oxides, pharmaceutically acceptable salts or deuterated analogs
substitution is restricted



CAS 科学家对文献多维度标引，快速获取研究重点

着重关注文献中涉及药理活性研究的物质，助力构效关系分析

Pharmacological Data 药理活性数据

Ligand	Target	Function	Parameter	Value	Disease	Organism	Assay
2820500-78-3	Epidermal growth factor receptor	Inhibitor	DC50	0.0033 μM	disease of cellular proliferation	-	View Detail
2820500-67-0	Epidermal growth factor receptor	Inhibitor	DC50	0.0027 μM	disease of cellular proliferation	-	
2820499-28-1	Epidermal growth factor receptor	Inhibitor	DC50	0.01043 μM	disease of cellular proliferation	-	
2820499-28-1	Epidermal growth factor receptor	Inhibitor	DC50	0.02496 μM	disease of cellular proliferation	-	
2820499-53-2	Epidermal growth factor receptor	Inhibitor	DC50	0.0054 μM	disease of cellular proliferation	-	
2820499-53-2	Epidermal growth factor receptor	Inhibitor	DC50	0.00895 μM	disease of cellular proliferation	-	
2820500-65-8	Epidermal growth factor receptor	Inhibitor	DC50	0.0043 μM	disease of cellular proliferation	-	
2820500-68-1	Epidermal growth factor receptor	Inhibitor	DC50	0.0018 μM	disease of cellular proliferation	-	
2820500-47-6	Epidermal growth factor receptor	Inhibitor	DC50	0.003 μM	disease of cellular proliferation	-	
2820500-54-5	Epidermal growth factor receptor	Inhibitor	DC50	0.0044 μM	disease of cellular proliferation	-	
2820499-40-7	Epidermal growth factor receptor	Inhibitor	DC50	0.5461 μM	disease of cellular proliferation	-	
2820499-40-7	Epidermal growth factor receptor	Inhibitor	DC50	0.1856 μM	disease of cellular proliferation	-	
2820500-53-4	Epidermal growth factor receptor	Inhibitor	DC50	0.0015 μM	disease of cellular proliferation	-	
2820499-34-9	Epidermal growth factor receptor	Inhibitor	DC50	0.03016 μM	disease of cellular proliferation	-	

Assay Data

Target	Epidermal growth factor receptor
Assay Name	-
Procedure	HTRE assay
Assay Comment	-
Condition	-
Parameter	DC50
Value	0.0027 μM
Measurement Remarks	-
Ligand Dose	-
Biological System	in vitro; H1975-clone-DTC; Cell with Del 19/T790M/C797S; Human
Source	Preparation of EGFR inhibitor-E3 ubiquitin ligase ligand conjugates as targeted degraders for treatment of cancer Inventors: Lei, Bailin; Liu, Huaqing; Han, Songzhe; Wang, Zhiwei World Intellectual Property Organization WO2022171123 A1 2022-08-18 Language: English, Database: CAplus

实验详情

重点回顾

CAS 科学家深度解析 Markush 结构

CAS SciFinder 科学家深入拆解读 Markush 结构，支持直观查阅 Markush 结构详情，助力可专利性评估；CAS 科学家对文献多维度标引，直接获取同族专利、权利要求、核心研究点、重要物质与反应以及药理毒理数据，节省阅读原文的时间

大纲

- 美国化学文摘社（CAS）与 CAS SciFinder Discovery Platform 简介
- AI 应用助力快速发现目标研究信息
- CAS 加强对专利信息挖掘的支持
- 全面开放生命科学领域数据与表征信息

药理数据连接药物结构与生物活性

Pharmacological Data

CAS LIFE SCIENCES

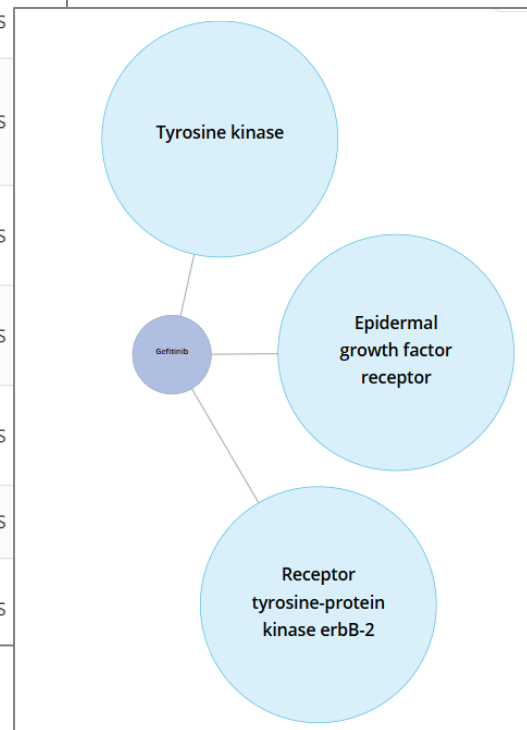
Clear All Filters Knowledge Graph

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Epidermal growth factor receptor		Selectivity	0.053	lung non-small cell carcinoma	Homo sapiens	View Detail	(1) CAS
Epidermal growth factor receptor		Protein phosphorylation	Significantly decreased epidermal growth factor receptor phosphorylation observed	lung non-small cell carcinoma	Homo sapiens	View Detail	(2) CAS
Epidermal growth factor receptor		Protein phosphorylation	Significant reduction in phosphorylation level observed	disease of cellular proliferation	Homo sapiens	View Detail	(3) CAS
Epidermal growth factor receptor	Inhibitor	Protein phosphorylation	No significant change in phosphorylation level observed	disease of cellular proliferation	Homo sapiens	View Detail	(3) CAS
Epidermal growth factor receptor	Inhibitor	Protein phosphorylation	No significant change in phosphorylation level observed	disease of cellular proliferation	Homo sapiens	View Detail	(3) CAS
Epidermal growth factor receptor	Inhibitor	Protein phosphorylation	Complete inhibition in phosphorylation observed	disease of cellular proliferation	Homo sapiens	View Detail	(3) CAS
Epidermal growth factor receptor	Inhibitor	Protein phosphorylation	Significant reduction in phosphorylation level observed	disease of cellular proliferation	Homo sapiens	View Detail	(3) CAS

Filter Target

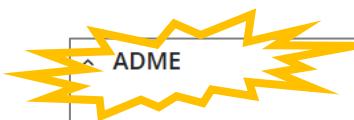
- Epidermal growth factor receptor (239)
- Tyrosine kinase (25)
- Receptor tyrosine-protein kinase erbB-2 (17)
- GTPase KRas (13)
- Proto-oncogene

Clear Apply



CAS SciFinder 可查询全面药理信息，便捷确认活性药物，科研更高效

药物代谢信息助力药代动力学研究评估



ADME
CAS LIFE SCIENCES

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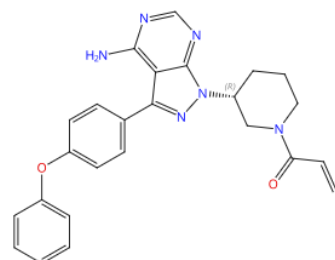
Target	Function	Parameter	Value	Disease
UDP-glucuronosyltransferase	Inhibitor	MRT (0-infinity)	23.95 hr	viral infectious disease
ATP-dependent translocase ABCB1	Inhibitor	P_{app (A-B)}	2.2 × 10 ⁻⁵ cm/s	rheumatoid arthritis; Parkinson's disease; Alzheimer's disease
ATP-dependent translocase ABCB1	Inhibitor	P_{app (B-A)}	3 × 10 ⁻⁶ cm/s	rheumatoid arthritis; Parkinson's disease; Alzheimer's disease
Tyrosine-protein kinase BTK	Inhibitor	Plasma concentration (free)	Reached C _{max} after 2 hours post administration and maintained at relatively stable level	central nervous system lymphoma
Tyrosine-protein kinase BTK	Inhibitor	Plasma concentration (free)	Reached C _{max} after 2 hours post administration and maintained at relatively stable level	central nervous system lymphoma

Assay Data CAS LIFE SCIENCES

← Prev (1 of 6) Next →

Target	Value
UDP-glucuronosyltransferase	23.95 hr
Assay Name	LC-MS
Procedure	LC-MS/MS assay
Assay Comment	-
Parameter	MRT (0-infinity)
Value	23.95 hr
Measurement Remarks	-
Ligand Dose	100 mg/kg
Route of Administration	Intraperitoneal
Condition Type	Drug interactions
Condition Material	Penindolone
Condition Value	3.5 mg/kg
Biological System	in vivo; Plasma; Rat; Sprague-dawley
Source	Biotransformation of Penindolone, an Influenza A Virus Inhibitor By: Liu, Shuai; Zheng, Keming; Jiang, Yilin; Gai, Susu; Li, Bohan; Li, Dehai; Yang, Shuang; Lv, Zhihua

Ligand 936563-96-1



Absolute stereochemistry shown

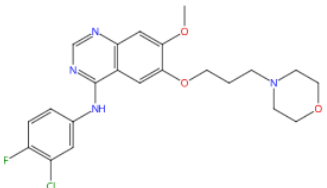
C₂₅H₂₄N₆O₂
Ibrutinib

药物代谢信息放开，提前判断成药性，节约合成资源

毒理信息助力安全评估、毒理研究与制剂开发



Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Salmonella typhimurium TA98	-	Mutagenicity	Negative	lung non-small c			
Salmonella typhimurium TA1537	-	Mutagenicity	Negative	lung non-small c			
Salmonella typhimurium TA1535	-	Mutagenicity	Negative	lung non-small c			
Salmonella typhimurium TA100	-	Mutagenicity	Negative	lung non-small c			
Human coronavirus OC43	-	Toxicity	0	COVID-19			
Human coronavirus OC43	-	Toxicity	0	COVID-19			
Epidermal growth factor receptor	Inhibitor	LC50	0.03144 μM	disease of cellu			

Assay Data	
Ligand 184475-35-2	Target Salmonella typhimurium TA98
	Assay Name Ames test
<chem>C22H24ClFN4O3</chem> Gefitinib	Procedure Mutagenicity was measured in Salmonella typhimurium TA98 upon incubation with compound at a concentration of 5 to 100 μM using Ames test.
	Assay Comment -
	Parameter Mutagenicity
	Value Negative
	Measurement Remarks -
	Ligand Dose 5-100 μM
	Route of Administration -
	Toxicity Type Genotoxicity
	Biological System in vitro
	Source Discovery of a Hydroxylamine-Based Brain Penetrant EGFR Inhibitor for Metastatic Non-Small-Cell Lung Cancer By: Hill, Jarvis; Jones, Robert M.; Crich, David World Intellectual Property Organization WO2022032113 A1 2022-02-10 Language: English,

毒理数据放开，Ames 试验，LD50 等数据助力毒理研究与制剂开发

新增多种实验数据，助力化合物表征结果分析

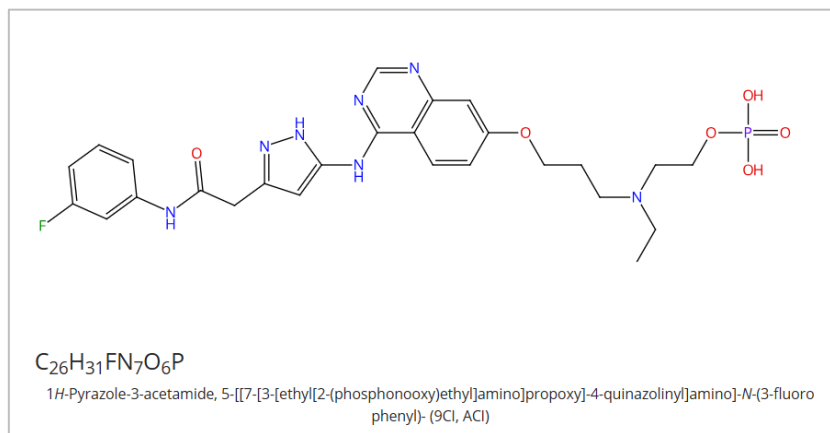
Experimental Properties										
Biological	Chemical	Density	Electrical	Flow and Diffusion	Interface	Lipinski	Mechanical	Optical and Scattering	Structure Related	Thermal
Property ∇		Value		Condition		Source				
Median Lethal Dose		2630 mg/kg		Organism: mouse; Route: intraperitoneal		(1) CAS				

Experimental Properties										
Biological	Chemical	Density	Electrical	Flow and Diffusion	Interface	Lipinski	Mechanical	Optical and Scattering	Structure Related	Thermal
Property ∇		Value		Condition		Source				
Electric Dipole Moment		6.6 D		-		(1) CAS				

Experimental Properties										
Biological	Chemical	Density	Electrical	Flow and Diffusion	Interface	Lipinski	Mechanical	Optical and Scattering	Structure Related	Thermal
Property ∇		Value		Condition		Source				
Critical Point		790.91 K, 4.419 x 10 ⁶ Pa		-		(1) CAS				
Critical Point		783 K		-		(2) CAS				
Formation Enthalpy		-1164.6 kJ/mol		-		(3) CAS				

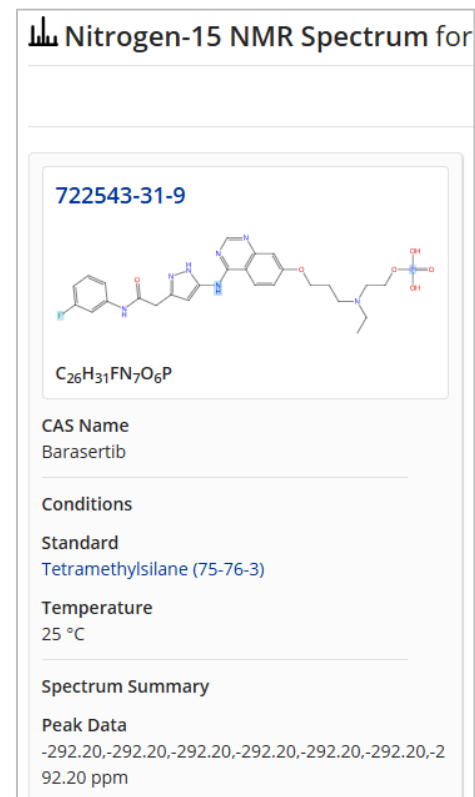
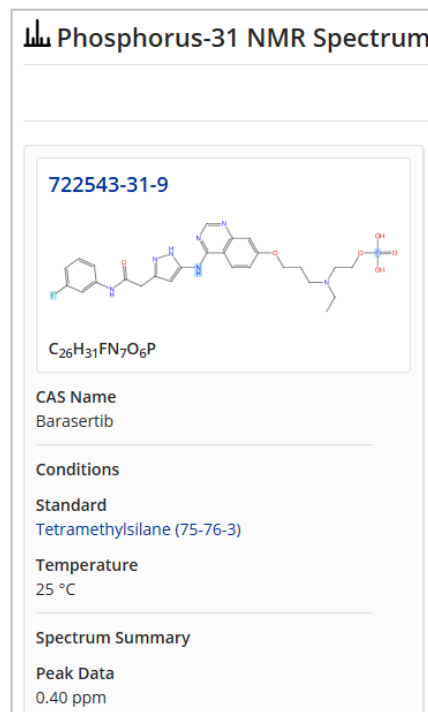
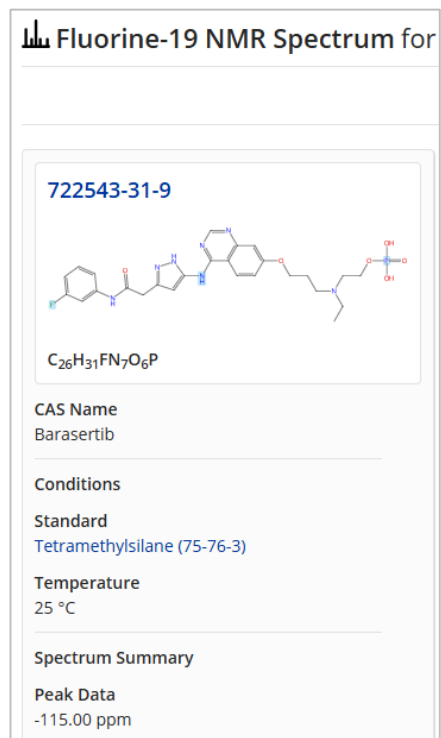
整合更多跨学科实验数据，助力化合物全方位表征分析与溯源

新增预测的杂原子核磁数据，助力化合物表征参考



新增 F-19、P-31 和 N-15 预测核磁数据
助力表征物质结构

注：针对包含F\N杂原子的小分子
(含金属物质、季铵盐无预测核磁数据)



为结构确证提供数据参考

重点回顾

全面开放生命科学领域数据与表征信息

CAS SciFinder 提供丰富的药理、药代与毒理信息，新增多种实验表征数据和预测杂原子核磁信息，助力结构表征，挖掘课题研究价值

Between problems
and progress **are**
connections that
matter

谢谢!

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