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爱思唯尔生命科学客户顾问



# 今天的内容

- 文献检索的原理简介
- Reaxys数据库**文献**检索的技巧
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- Reaxys数据库**专利**检索技巧
  - NASH(Nonalcoholic steatohepatitis)治疗相关的专利检索
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- Reaxys Medicinal Chemistry**数据**检索技巧
  - 如何通过靶点筛选小分子抑制剂

# 文献信息检索的挑战



1. 使用什么‘检索词汇’进行检索？
2. 为什么‘检索词汇’输入后，得到了‘这个结果’？
3. 检索结果如何更便捷的查看？



1. 怎么检索不到？这么检索这么少？怎么检索这么多？
2. 如何缩小范围？如果扩大范围？
3. 如何分类，如何整理？

# 什么是检索词汇

Free text

标题

**Non-oncogenic Acute Viral Infections Disrupt Anti-cancer Responses and Lead to Accelerated Cancer-Specific Host Death**

作者关键词

摘要

SUMMARY

In light of increased cancer prevalence and cancer-specific deaths in patients with infections, we investigated whether infections alter anti-tumor immune responses. We report that acute influenza infection of the lung promotes distal melanoma growth in the dermis and leads to accelerated cancer-specific host death. Furthermore, we show that during influenza infection, anti-melanoma CD8<sup>+</sup> T cells are shunted from the tumor to the infection site, where they express high levels of the inhibitory receptor programmed cell death protein 1 (PD-1). Immunotherapy to block PD-1 reverses this loss of anti-tumor CD8<sup>+</sup> T cells from the tumor and decreases infection-induced tumor growth. Our findings show that acute non-oncogenic infection can promote cancer growth, raising concerns regarding acute viral illness sequelae. They also suggest an unexpected role for PD-1 blockade in cancer immunotherapy and provide insight into the immune response when faced with concomitant challenges.

Index term

正文核心词汇

discordant

anti-tumor

programmed cell death protein 1

Influenza infection

Cell Reports  
Report

OPEN  
ACCESS  
CellPress

**Non-oncogenic Acute Viral Infections Disrupt Anti-cancer Responses and Lead to Accelerated Cancer-Specific Host Death**

Frederick J. Kohlhapp,<sup>1,2,3,4</sup> Erica J. Huelsmann,<sup>5,11</sup> Andrew T. Loock,<sup>6,11</sup> Jason M. Schankel,<sup>4,11</sup> Jevgeniya Lusciuk,<sup>2,4</sup> Joseph R. Brucsek,<sup>2</sup> Josef W. Goldofsky,<sup>2</sup> Tasha Hughes,<sup>2</sup> Janet P. Zayas,<sup>2</sup> Hubert Dolukhaino,<sup>2</sup> Ryan T. Sowell,<sup>2</sup> Regina Kufner,<sup>2</sup> Sarah Burd,<sup>7</sup> John C. Kubacki,<sup>8</sup> Arman Nabatiyan,<sup>1,9</sup> ShyRae Marshall,<sup>1</sup> Praveen K. Sommareddy,<sup>1</sup> Shanoguo Li,<sup>1</sup> Jenna H. Newman,<sup>1</sup> Claude E. Monkton,<sup>1,2</sup> Satha H. Shafiqhani,<sup>2</sup> Amanda L. Marzo,<sup>2,4</sup> Jose A. Guevara-Palino,<sup>2</sup> Ahmed Laafar,<sup>1,8</sup> Paul G. Thomas,<sup>10</sup> Edmund C. Lattima,<sup>1,2</sup> Howard L. Kaufman,<sup>1,2</sup> and Andrew Zozor<sup>1,2,3,4</sup>

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<http://dx.doi.org/10.1016/j.celrep.2016.09.068>

SUMMARY

In light of increased cancer prevalence and cancer-specific deaths in patients with infections, we investigated whether infections alter anti-tumor immune responses. We report that acute influenza infection of the lung promotes distal melanoma growth in the dermis and leads to accelerated cancer-specific host death. Furthermore, we show that during influenza infection, anti-melanoma CD8<sup>+</sup> T cells are shunted from the tumor to the infection site, where they express high levels of the inhibitory receptor programmed cell death protein 1 (PD-1). Immunotherapy to block PD-1 reverses this loss of anti-tumor CD8<sup>+</sup> T cells from the tumor and decreases infection-induced tumor growth. Our findings show that acute non-oncogenic infection can promote cancer growth, raising concerns regarding acute viral illness sequelae. They also suggest an unexpected role for PD-1 blockade in cancer immunotherapy and provide insight into the immune response when faced with concomitant challenges.

made to the immune system. Such work has been instrumental in discerning the complex interactions between host and intracellular molecular signaling networks. However, the immune system is often tasked with responding to multiple concomitant challenges, and how one type of challenge affects the immune response to another is not well understood.

The majority of the work thus far on concomitant challenges has been done in the context of pathogenic co-infections, and findings in this field are discordant (Kinney et al., 2015; Mueller et al., 2007; Osborne et al., 2014; Shrikant et al., 2014). Further, although infections and cancers are two of the most common human maladies and cancer patients are at increased risk of infections, very little information regarding the consequences of concomitant non-oncogenic infection and cancer; thus, this subject is a matter of ongoing debate (Coolieley et al., 2005; Kohler et al., 1990; Wong et al., 2010). Case studies performed in the late 19<sup>th</sup> century report cancer regression in the context of infection-like reactions (e.g., in response to Coley's toxin), and recent work proposes that anti-tumor T cell populations can be expanded as a by-product of infection (Coley, 1891; Ganett, 2015; Inagawa et al., 2014). However, emerging epidemiological studies report an increased prevalence of cancers and increased cancer incidence (Attkin et al., 2014; Cox et al., 2010; Crum-Ganfone et al., 2009; Huang et al., 2011; Swaminathan et al., 2013).

INTRODUCTION

Our current understanding of immunity relies principally on studies in which a single type of challenge or re-challenge is

Therefore, toward advancing the scientific understanding of immunity in the context of multiple concomitant challenges, we investigated the effect of acute, non-oncogenic,



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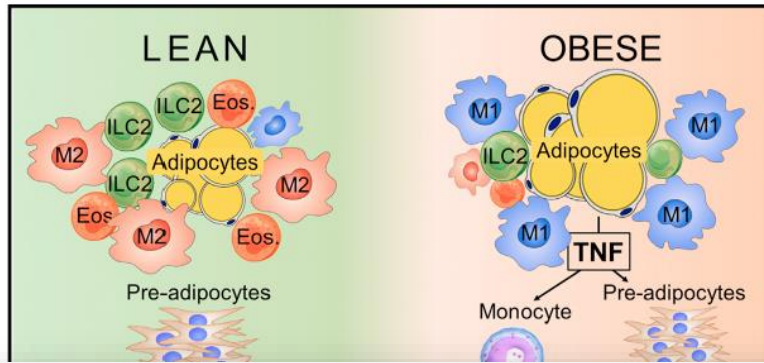
# 什么是同义词

## Cell Reports

Report

### PD-1 Is Involved in the Dysregulation of Type 2 Innate Lymphoid Cells in a Murine Model of Obesity

Graphical Abstract



Authors

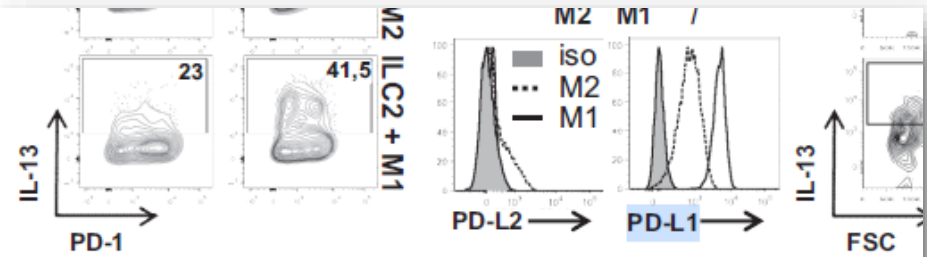
Guillaume Oldenhove, Elodie Boucquey, Anaëlle Taquin, ..., Kevin Englebert, Louis Boon, Muriel Moser

Correspondence

guillaume.oldenhove@ulb.ac.be

In Brief

The function of ILC2s is compromised during obesity. Here, Oldenhove et al.



correlation between PD-1 expression, ILC2 dysfunction, and consequently impaired beige adipocyte function (Figures 1E and S3). By contrast, KLRG1 was expressed by all ILC2s in both lean and obese mice, and ICOS was slightly upregulated in a minor population of ILC2s, regardless of PD-1 expression (Figure 1D).

#### M1-type Macrophages Express PD-L1 and Inhibit ILC2 Function In Vitro

We next examined whether the expression of the PD-L1 was also regulated in the visceral adipose tissue during chronic inflammation. The data in Figure 2A show that MHCII<sup>+</sup> CD64<sup>+</sup> cells, which mainly represent macrophages (Tamoutounour et al., 2012), displayed increased levels of PD-L1 in WT obese mice. Of note, two

1 PD-1 Is Involved in the Dysregulation of Type 2 Innate Lymphoid Cells in a Murine Model of Obesity

Oldenhove G., Boucquey E., Taquin A., Acolty V., Bonetti L., Ryffel B., Le Bert M., Englebert K., Boon L., Moser M.

Cell Reports 2018 25:8 (2053-2060.e4) Cited by: 5

Embase MEDLINE [Abstract](#) [Index Terms](#) [View Full Text](#)

Abstract:

Recent observations clearly highlight the critical role of type 2 innate lymphoid cells in maintaining the indirectly by sustaining a Th2-prone environment enriched in eosinophils and alternatively activated macrophages in obese individuals. In this work, we identify the PD-1-PD-L1 pathway as a factor leading to ILC2 destabilization and triggering interleukin-33 (IL-33)-dependent PD-1 expression on ILC2s and recruiting and activating PD-1<sup>hi</sup> ILC2s. The function of ILC2s is compromised during obesity. Here, Oldenhove et al. show that ILC2s promote type 2 innate responses, and promoted tissue homeostasis. PD-1 may therefore represent a target for immunomodulation.

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1 PD-1 Is Involved in the Dysregulation of Type 2 Innate Lymphoid Cells in a Murine Model of Obesity

Oldenhove G., Boucquey E., Taquin A., Acolty V., Bonetti L., Ryffel B., Le Bert M., Englebert K., Boon L., Moser M. Cell Reports 2018 25:8 (2053-2060.e4) Cited by: 5

Embase MEDLINE [Abstract](#) [Index Terms](#) [View Full Text](#)

Drug Terms

interleukin 1 receptor like 1 protein<sup>®</sup>, interleukin 33<sup>®</sup>, messenger RNA<sup>®</sup>, programmed death 1 ligand 1<sup>®</sup>, transmembrane protein<sup>®</sup>

Disease Terms

obesity<sup>®</sup>

Other Terms

adipose tissue<sup>®</sup>, animal cell<sup>®</sup>, animal experiment<sup>®</sup>, animal model<sup>®</sup>, article<sup>®</sup>, bone marrow cell<sup>®</sup>, cell differentiation<sup>®</sup>, eosinophil count<sup>®</sup>, glucose tolerance<sup>®</sup>, in vitro study<sup>®</sup>, intra-abdominal fat<sup>®</sup>, lipid diet<sup>®</sup>, lymphoid cell<sup>®</sup>, macrophage<sup>®</sup>, protein function<sup>®</sup>, upregulation<sup>®</sup>

# 检索词汇如何索引文献

标题 作者关键词

Non-oncogenic acute Viral Infections  
Disrupt Anti-tumor Immune Responses  
and Lead to Accelerated Cancer-Specific Host Death

摘要

**SUMMARY**  
In light of increased cancer prevalence and cancer-specific deaths in patients with infections, we investigated whether infections alter anti-tumor immune responses. We report that acute influenza infection of the lung promotes distal melanoma growth in the demis and leads to accelerated cancer-specific host death. Furthermore, we show that during influenza infection, anti-melanoma CD8<sup>+</sup> T cells are shunted from the tumor to the infection site, where they express high levels of the inhibitory receptor programmed death protein 1 (PD-1). Immunotherapy to block PD-1 reverses this loss of anti-tumor CD8<sup>+</sup> T cells and decreases infection-induced tumor growth. Our findings show that acute non-oncogenic infection can promote cancer growth, raising concerns regarding acute viral illness sequelae. They also suggest an unexpected role for PD-1 blockade in cancer immunotherapy and provide insight into the immune response when faced with concomitant challenges.

Free text

Index term

正文核心词汇

anti-tumor

discordant

program

death protein 1

Influenza infection

PD-1

- ‘free text’ 匹配是进行词汇的一致性匹配，不做扩展
- ‘index term’ 匹配是会包含同义词和下位词的匹配



检索词汇，进行 ‘free text’ 命中文献，进行 ‘index term’ 命中文献，再去重呈现结构



# 一篇全文期刊中的内容

Available 10/16/2019 12:19:26 PM

Contents lists available at ScienceDirect

**Tetrahedron**

Journal homepage: www.elsevier.com/locate/tet

**Assessment of the regioselectivity in the condensation reaction of unsymmetrical *o*-phthalaldehydes with alanine**

Agathe CA D'Hollander, Nicholas J Westwood\*

School of Chemistry and Biochemical Science, Brunel University, Uxbridge, Middlesex, UB8 3PH, UK; School of Chemistry, Brunel University, Uxbridge, Middlesex, UB8 3PH, UK

ARTICLE INFO

ABSTRACT

The approach for the synthesis of unsymmetrical *o*-phthalaldehyde isomers is discussed. The regioselectivity in the condensation reaction of unsymmetrical *o*-phthalaldehydes with alanine is assessed. The regioselectivity in the condensation reaction of unsymmetrical *o*-phthalaldehydes with alanine is assessed. The regioselectivity in the condensation reaction of unsymmetrical *o*-phthalaldehydes with alanine is assessed.

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1. Introduction

The introduction makes up an important part of a research paper. It should include the background information, the objectives of the study, and the significance of the work. It should also include a brief summary of the methods used and the results obtained. The introduction should be written in a clear and concise manner, and should be well organized and easy to read.

2. Results and discussion

The results and discussion section of a research paper is where the authors present their findings and discuss their implications. This section should be well organized and easy to read, and should include a clear and concise summary of the results and a discussion of their implications.

3. Conclusions

The conclusions section of a research paper is where the authors summarize their findings and provide a final statement on the significance of their work. This section should be well organized and easy to read, and should include a clear and concise summary of the results and a final statement on the significance of the work.

4. Acknowledgements

The acknowledgements section of a research paper is where the authors thank those who have helped them in their work. This section should be well organized and easy to read, and should include a clear and concise list of the names of those who have helped them.

5. References

The references section of a research paper is where the authors list the sources of the information they have used in their work. This section should be well organized and easy to read, and should include a clear and concise list of the references.

## 标题摘要

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## 数据, 原文关键词 (含同义词)

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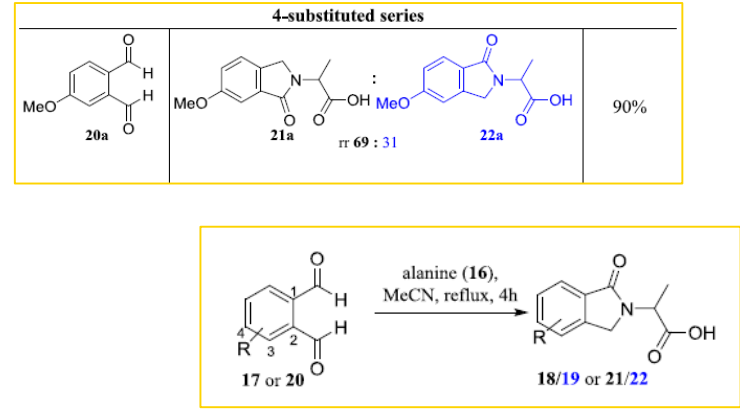
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## 支持信息



**21a: Mp:** 194–196 °C; IR  $\nu_{\text{max}}$  cm<sup>-1</sup> (thin film) 3370 (O–H stretch), 1730 (C=O stretch), 1636 (C=O stretch), 1493 (C=C stretch), 1456 (C–H bend), 1447 (C–H bend), 1196 (C–O stretch), 1022, 770; <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD)  $\delta_{\text{H}}$  7.48 (d, *J* = 8.5 Hz, 1H, H<sub>4</sub>), 7.29 (d, *J* = 2.5 Hz, 1H, H<sub>7</sub>), 7.19 (dd, *J* = 8.5, 2.5 Hz, 1H, H<sub>5</sub>), 5.00 (q, *J* = 7.5 Hz, 1H, CH), 4.54 (d, *J* = 17.0 Hz, 1H, H<sub>3</sub>), 4.48 (d, *J* = 17.0 Hz, 1H, H<sub>3</sub>), 3.86 (s, 3H, OCH<sub>3</sub>), 1.60 (d, *J* = 7.5 Hz, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD)  $\delta_{\text{C}}$  174.8 (COOH), 171.0 (C1), 161.6 (C6), 135.8 (C3a), 134.3 (C7a), 125.2 (C4), 121.0 (C5), 107.4 (C7), 56.1 (OCH<sub>3</sub>), 51.2 (CH), 48.1 (C3), 15.9 (CH<sub>3</sub>); HRMS (ES<sup>+</sup>) *m/z* calculated for C<sub>12</sub>H<sub>14</sub>NO<sub>4</sub> [M+H]<sup>+</sup>: 236.0917; found: 236.0921. See S11 part IX for experimental procedure and S12 for <sup>1</sup>H and <sup>13</sup>C NMR spectra.

**22a: Mp:** 191–193 °C; IR  $\nu_{\text{max}}$  cm<sup>-1</sup> (thin film) 3229 (O–H stretch), 1717 (C=O stretch), 1628 (C=O stretch), 1611 (C=C stretch), 1558 (C=C stretch), 1506 (C=C stretch), 1447 (C–H bend), 1435 (C–H bend), 1298 (C–N stretch), 1206 (C–O stretch), 1086, 1026, 845, 775; <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD)  $\delta_{\text{H}}$  7.68 (d, *J* = 8.5 Hz, 1H, H<sub>7</sub>), 7.13 (d, *J* = 2.0 Hz, 1H, H<sub>4</sub>), 7.04 (dd, *J* = 8.5, 2.2 Hz, 1H, H<sub>6</sub>), 4.98 (q, *J* = 7.5 Hz, 1H, CH), 4.57 (d, *J* = 17.0 Hz, 1H, H<sub>3</sub>), 4.50 (d, *J* = 17.0 Hz, 1H, H<sub>3</sub>), 3.88 (s, 3H, OCH<sub>3</sub>), 1.60 (d, *J* = 7.5 Hz, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD)  $\delta_{\text{C}}$  174.8 (COOH), 171.0 (C1), 164.9 (C5), 146.2 (C3a), 125.6 (C7), 125.4 (C7a), 116.3 (C6), 108.8 (C4), 56.2 (OCH<sub>3</sub>), 50.9 (CH), 48.4 (C3), 15.9 (CH<sub>3</sub>); HRMS (ES<sup>+</sup>) *m/z* calculated for C<sub>12</sub>H<sub>14</sub>NO<sub>4</sub> [M+H]<sup>+</sup>: 236.0917; found: 236.0921. See S11 part IX for experimental procedure and S12 for <sup>1</sup>H and <sup>13</sup>C NMR spectra.

inseparable regioisomers **28** and **29** in good yield (90%, 1.2 g). Derivatization using thionyl chloride and methanol gave the now separable regioisomeric esters isolated in 1.06 g for ester **30** (84% yield) and 0.2 g for ester **31** (16% yield) respectively. The overall esterification yield was quantitative and thus the initial ratio of **28** and **29** for the larger scale was calculated as 84:16 which was comparable to the small scale result (88:12 of **28:29**). Inspired by this result, the condensation reaction was attempted on a small scale (30 mg of **27**) at room temperature (as opposed to reflux) and led to an excellent regioselectivity of 97:3 of **28:29** (Scheme 3 and S11 part IV.3).

## 文献中包含的内容: 一些关键的概念

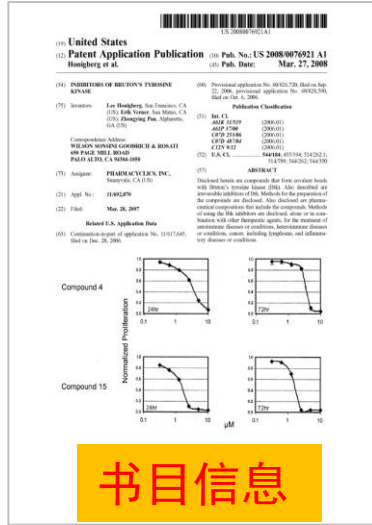
**2-(6-Methoxy-1-oxisoindolin-2-yl)propanoic acid (21a) via methyl 2-(bromomethyl)-5-methoxybenzoate (S43)**

**S43** was synthesised according to general procedure E using methyl 5-methoxy-2-methylbenzoate (**S41**, 1.00 equiv, 1.05 g, 5.8 mmol), NBS (1.10 equiv, 1.14 g, 6.4 mmol), AIBN (0.02 equiv, 0.02 g, 0.1 mmol) in CHCl<sub>3</sub> (24 mL). The reaction was refluxed for 21 h. Crude **S43** was treated according to general procedure L using alanine (**16**, 1.5 equiv, 775 mg, 8.7 mmol) and NEt<sub>3</sub> (2.2 equiv, 1.78 mL, 12.8 mmol). The reaction was refluxed for 2 h. Crude **21a** was basified using an aqueous solution of NaOH (2 M) and the organic impurities were extracted with DCM. The aqueous layer was acidified using an aqueous solution of HCl (1 M). The organics were extracted with DCM, combined, dried over MgSO<sub>4</sub> and concentrated *in vacuo*. Pure **21a** was obtained after titration in MeCN as a white solid (51 mg, 0.22 mmol, 49% over 2 steps). Characterisation of **21a** provided in the main paper and <sup>1</sup>H and <sup>13</sup>C NMR spectra of **21a** given in S12.

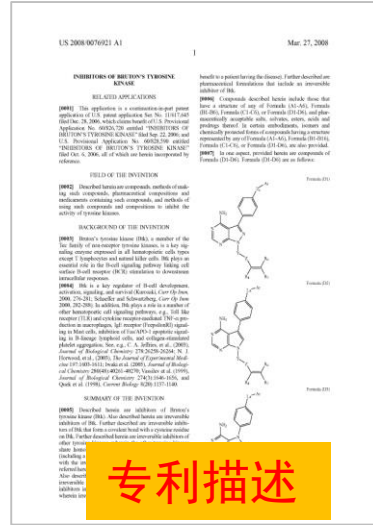
## Supporting Information 中的内容



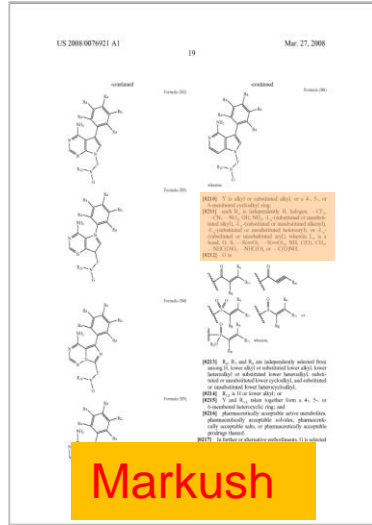
# 一篇典型的药物方面专利原文



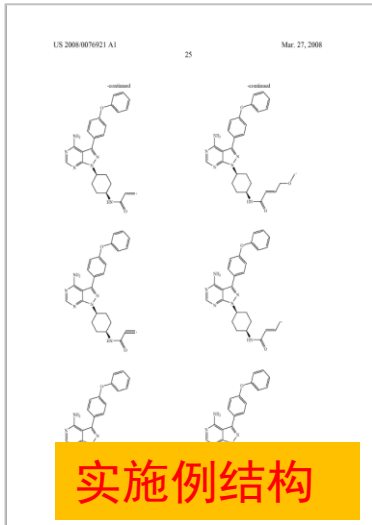
## 书目信息



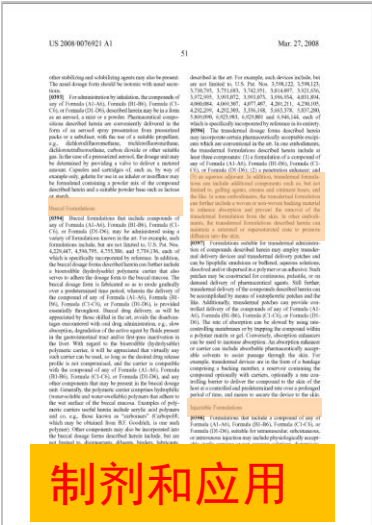
## 专利描述



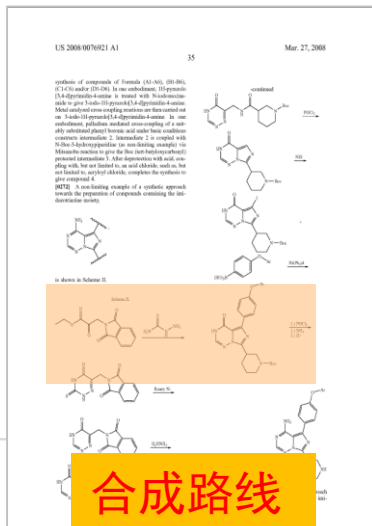
## Markush



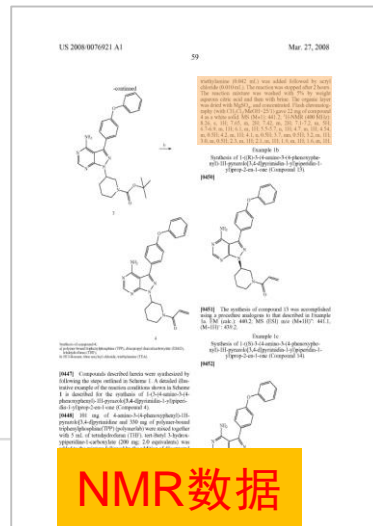
## 实施例结构



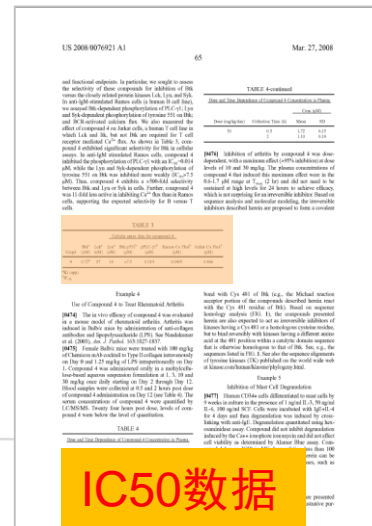
## 制剂和应用



## 合成路线



## NMR数据



## IC50数据

## 典型药物专利中的内容：

1. 书目内容
2. 专利描述
3. Markush结构及实施例
4. 反应合成路线
5. 实施例的实验室数据
6. 实施例的应用数据





# 今天的内容

- 文献检索的原理简介
- Reaxys数据库**文献**检索的技巧
  - Keytruda 相关信息检索
  - 中枢神经系统常见肿瘤分子病理学及靶向治疗
- Reaxys数据库**专利**检索技巧
  - NASH(Nonalcoholic steatohepatitis)治疗相关的专利检索
  - CD137相关的生物药专利
- Reaxys Medicinal Chemistry**数据**检索技巧
  - 如何通过靶点筛选小分子抑制剂



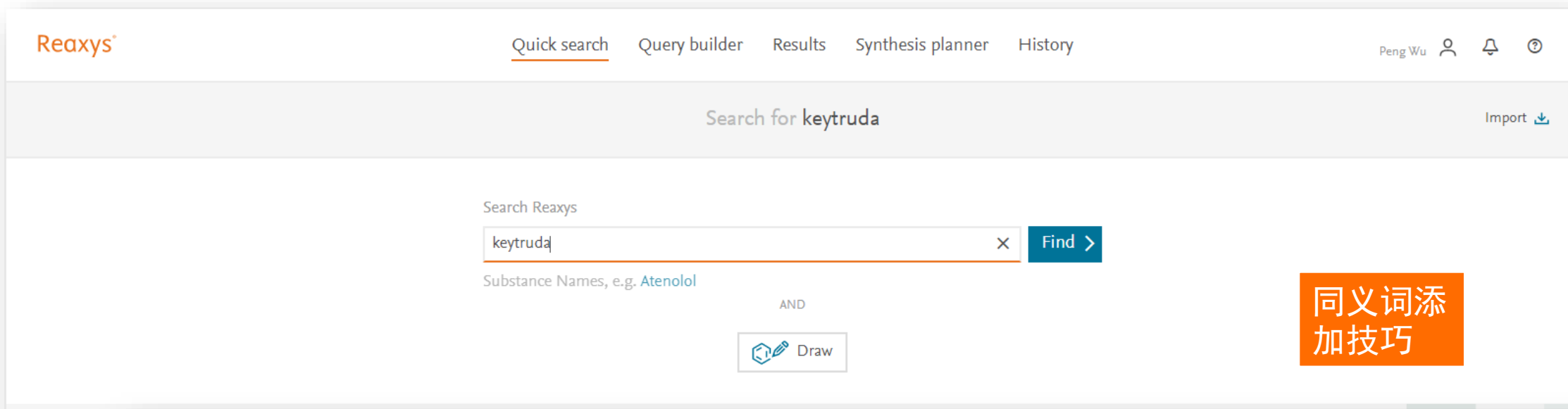
## Reaxys文献检索技巧

**Case 1: Keytruda 相关信息检索**

**Case 2: 中枢神经系统常见肿瘤分子病理学及靶向治疗**



# Case 1: Keytruda相关信息检索



Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Peng Wu

Search for keytruda Import

Search Reaxys

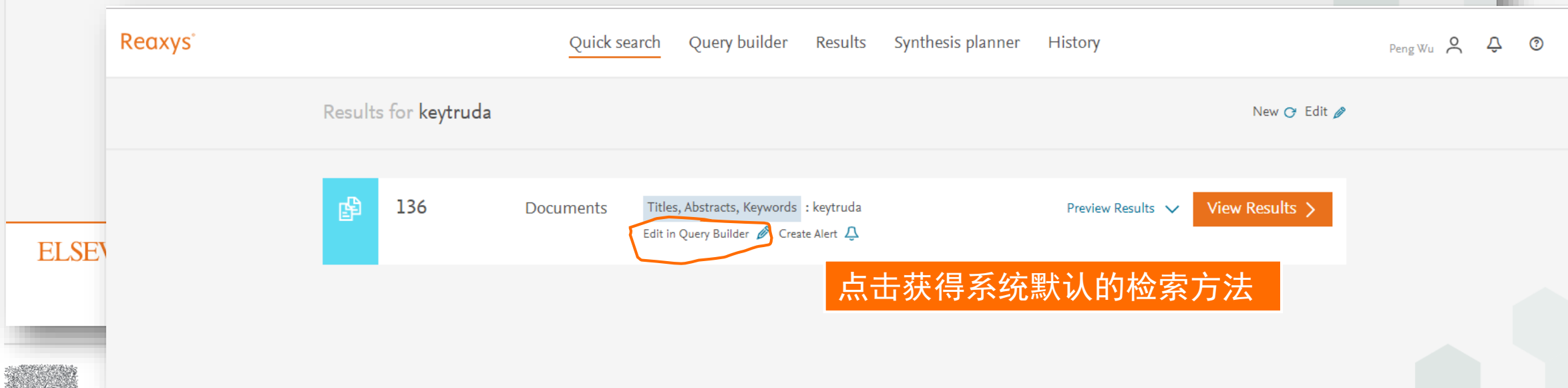
keytruda × Find >

Substance Names, e.g. Atenolol

AND

Draw

同义词添加技巧



Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Peng Wu

Results for keytruda New Edit

136 Documents Titles, Abstracts, Keywords : keytruda Preview Results View Results >

Edit in Query Builder Create Alert

点击获得系统默认的检索方法



Search in:

Reactions &gt;

Targets &gt;

Substances &gt;

Documents &gt;

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

; 此符号表达 'or' 逻辑关系

Titles, Abstracts &amp; K...

is

keytruda;keytruda;Pembrolizumab

添加同义词

🔍 ✕

## Filters

Limit to &gt;

Exclude &gt;

Index Terms (List) ▾

Index Terms (ReaxysTree) ▾

Publication Year ▾

Document Type ▾

Authors ▾

Patent Assignee ▾

Journal Title ▾

Substance Classes ▾

Reaction Classes ▾

7,678 Documents with 26,980 Substances, 36,630 Reactions, 332 Targets

 0 selected Limit To Exclude Export

🔍 🔍

Sort by Publication Year ↓ ▾

Heatmap 🗃

 Regressed melanocytic nevi secondary to pembrolizumab therapy: an emerging melanocytic dermatologic effect from immune checkpoint antibody blockade Cited 4 times

1  
Mauzo, Shakuntala H.; Tetzlaff, Michael T.; Nelson, Kelly; Amaria, Rodabe; Patel, Sapna; Aung, Phyu P.; Nagarajan, Priyadharsini; (...)  
Prieto, Victor G.; Curry, Jonathan L. [International Journal of Dermatology, 2019, vol. 58, # 9, p. 1045 - 1052]

Abstract ▾ Index Terms ▾ Substances 5 ▾ Full Text ↗

Index Terms hit: {...monoclonal antibody HMB 45, pembrolizumab, prednisone...}

 Thoracic Imaging of Non-Small Cell Lung Cancer Treated With Anti-programmed Death Receptor-1 Therapy Cited 3 times

2  
Hammer, Mark; Bagley, Stephen; Aggarwal, Charu; Bauml, Joshua; Nachiappan, Arun C.; Simone, Charles B.; Langer, Corey; Katz, Sharyn I.  
[Current Problems in Diagnostic Radiology, 2019, vol. 48, # 2, p. 142 - 147]

Abstract ▾ Index Terms ▾ Full Text ↗

Index Terms hit: {...nivolumab, pembrolizumab, programmed death 1 receptor...}

多种筛选器便于筛选文章



ELSEVIER

Index Terms (List)	▼
Index Terms (ReaxysTree)	▼
Publication Year	▼
Document Type	▼
Authors	▼
Patent Assignee	▼
Journal Title	▼
Substance Classes	▼
Reaction Classes	▼

### Document Type

<input type="checkbox"/> review	2,870
<input type="checkbox"/> article	2,656
<input type="checkbox"/> patent	795
<input type="checkbox"/> note	403
<input type="checkbox"/> editorial	327
<input type="checkbox"/> letter	319
<input type="checkbox"/> short survey	133

[View more](#)

### Publication Year

<input type="checkbox"/> 2019	1,769
<input type="checkbox"/> 2018	2,256
<input type="checkbox"/> 2017	1,800
<input type="checkbox"/> 2016	1,141
<input type="checkbox"/> 2015	573
<input type="checkbox"/> 2014	138
<input type="checkbox"/> 2013	1

[Filter by value](#) ▼

### Journal Title

<input type="checkbox"/> journal for immunothera...	141
<input type="checkbox"/> immunotherapy	119
<input type="checkbox"/> annals of oncology	118
<input type="checkbox"/> clinical cancer research	107
<input type="checkbox"/> oncotarget	105
<input type="checkbox"/> journal of thoracic oncol...	102
<input type="checkbox"/> european journal of cancer	100

[Filter by value](#) ▼ [View more](#)

可直接数据词汇进行筛选，如‘Lancet’

Search in: [Reactions >](#) [Targets >](#) [Substances >](#) [Documents >](#)

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

◇ Titles, Abs

◇ Titles, Abs

AND

248 Documents with 1,644 Substances, 2,309 Reactions, 12 Targets

0 selected [Limit To](#) [Exclude](#) [Export](#)

Sort by Relevance ↓ [Heatmap](#)

FDA approval summary: **Pembrolizumab** for the treatment of patients with unresectable or metastatic melanoma [Cited 16 times](#)

[Barone, Amy](#); [Hazarika, Maitreyee](#); [Theoret, Marc R.](#); [Mishra-Kalyani, Pallavi](#); [Chen, Huanyu](#); [He, Kun](#); [Sridhara, Rajeshwari](#); (...) [Keegan, Patricia](#); [Pazdur, Richard](#) [Clinical Cancer Research, 2017, vol. 23, # 19, p. 5661 - 5665]

[Abstract](#) [Index Terms](#) [Substances 2](#) [Full Text](#)

Abstract hit: {...approval to **pembrolizumab** (KEYTRUDA; Merck Sharp & Dohme Corp.) for treatment of patients...}

Index Terms

EMTREE drug term: carboplatin, dacarbazine, ipilimumab, paclitaxel, **pembrolizumab**, temozolomide

EMTREE medical term: adolescent, adult, aged, antineoplastic activity, area under the curve, Article, cancer survival, constipation, controlled study, decreased appetite, diarrhea, drug clearance, drug determination, drug distribution, drug dose escalation, drug efficacy, drug half life, drug safety, fatigue, human, hyperthyroidism, hypothyroidism, major clinical study, metastatic melanoma, middle aged, multicenter study, nausea, overall survival, pneumonia, priority journal, progression free survival, randomized controlled trial, rash, very elderly, young adult

Reaxys Index Terms: area under the curve, clearance, pharmacokinetic, **pharmacological** property, plasma concentration, toxicity

Clinical **pharmacologic** aspects of immune checkpoint inhibitors in cancer therapy

[Kim, Kyu-Pyo](#); [Jung, Hun](#) [Translational and Clinical Pharmacology, 2016, vol. 24, # 1, p. 7 - 12]

相关关键词





# Case 2: 中枢神经系统常见肿瘤分子病理学及靶向治疗

Reaxys® Quick search Query builder Results Synthesis planner History Peng Wu

Search for Molecular Pathology and Targeted Therapy of Common Tumors in the Central Nervous System Import

Search Reaxys

Molecular Pathology and Targeted Therapy of Common Tumors in the Central Nervous System X Find >

Cell Lines Name, e.g. HEK293

AND

Draw

主题检索的难点在于，如何拆分关键词，如何构建检索逻辑，如何选取同义词

直接复制主题句子进行检索

Reaxys® Quick search Query builder Results Synthesis planner History Peng Wu

Results for Molecular Pathology and Targeted Therapy of Common Tumors in the Central Nervous System New Edit

8 Documents

Titles, Abstracts, Keywords : "Molecular Pathology", "Targeted", "Therapy", "Common", "Tumors", "Central Nervous System"

Edit in Query Builder Create Alert

Preview Results View Results >

一键获取默认检索逻辑

# 手动调节，控制检索文献的范围，精确度

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

系统默认检索逻辑

手动添加或减少同义词

改变关键词间逻辑关系

◇ Titles, Abstracts & K...	is	▼	"molecular etiology";"molecular pathogenesis";"molecular pathology";"molecular pathophysiology";"pathology, molecular"	🔍	✕
◇ Titles, Abstracts & K...	is	▼	"targeted"	🔍	✕
◇ Titles, Abstracts & K...	is	▼	"Therapy"	🔍	✕
◇ Titles, Abstracts & K...	is	▼	"tumors"	🔍	✕
◇ Titles, Abstracts & K...	is	▼	"c.n.s."; "central nerve system"; "central nervous system"; "cns"; "nervous system, central"; "neural analyzers"; "systema nervosum c"	🔍	✕
◇ Titles, Abstracts & K...	is	▼	Common	🔍	✕

Search in:

Reactions &gt;

Targets &gt;

Substances &gt;

Documents &gt;

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

◇ Titles, Abstracts & K... is ▾ "molecular etiology";"molecular pathogenesis";"molecular pathology";"molecular pathophysiology";"pathology, molecular" 𐀀 ✕

AND

Group 1 𐀀 Ungroup

定义两个关键词之间间隔1-3

◇ Titles, Abstracts & K... is ▾ "targeted" 𐀀 ✕

NEAR 3

◇ Titles, Abstracts & K... is ▾ "Therapy" 𐀀 ✕

AND

◇ Titles, Abstracts & K... is ▾ "c.n.s."; "central nerve system"; "central nervous system"; "cns"; "nervous system, central"; "neural analyzers"; "systema nervosum c" 𐀀 ✕

AND

◇ Titles, Abstracts & K... is ▾ tumor;cancer 𐀀 ✕



27 Documents with 39 Substances, 0 Reactions, 1 Targets

0 selected Limit To Exclude Export

结果集也被扩大

Sort by Publication Year ↓ Heatmap

Molecular pathogenesis and therapeutic implications in pediatric high-grade gliomas

儿童高级别胶质瘤的分子发病机制及治疗意义

1 Juratli, Tareq A.; Qin, Nan; Cahill, Daniel P.; Filbin, Mariella G. [Pharmacology and Therapeutics, 2018, vol. 182, p. 70 - 79]

Abstract ^ Index Terms ^ Substances 10 v Full Text ↗

#### Abstract

High-grade gliomas (HGG) are the most common malignant brain tumors in the pediatric population and account for a large subset of all pediatric central nervous system neoplasms. The management of pediatric HGG continues to be challenging, with poor outcome in many cases despite aggressive treatments. Consequently, parallel research efforts have been focused on identifying the underlying genetic and biological basis of pediatric HGG in order to more clearly define prognostic subgroups for treatment stratification as well as identify new treatment targets. These cutting-edge advances have revolutionized pediatric neuro-oncology and have revealed novel oncogenic vulnerabilities that are being therapeutically leveraged. Promising treatments – including pathway-targeting small molecules as well as epigenetic therapy – are being evaluated in clinical trials, and recent genomic discoveries in rare glioma subgroups have led to the identification of additional new potentially-actionable alterations. This review summarizes the current state of knowledge about the molecular characterization of pediatric HGG in correlation to the revised World Health Organization (WHO) classification, as well as provides an overview of some targeted treatment approaches in the modern clinical management of high-grade gliomas.

#### Index Terms

**Author keyword:** Brain tumor, CNS, Epigenetics, IDH, Pediatric glioma, Targeted therapy

**EMTREE drug term:** histone H3

**EMTREE medical term:** anaplastic ganglioglioma, antiangiogenic activity, cancer patient, cancer prognosis, cancer staging, cancer survival, carcinogenesis, child, childhood cancer, disease association, gene mutation, gene targeting, genetic code, glioblastoma, glioma, human, malignant transformation, missense mutation, molecular pathology, molecularly targeted therapy, outcome assessment, overall survival, pleomorphic xanthoastrocytoma, pontine glioma, priority journal, Review, somatic mutation, world health organization

**Reaxys Index Terms:** Permeability, acetylation, domain boundary, maximum tolerated dose, methylation, separation method, transfer reaction

Epithelioid hemangioendothelioma as a model of YAP/TAZ-driven cancer: Insights from a rare fusion sarcoma

Cited 3 times

2 Lamar, John M.; Nehru, Vijeyaluxmy Motilal; Weinberg, Guy [Cancers, 2018, vol. 10, # 7, art. no. 229]



## Reaxys专利检索技巧

**Case 3: NASH(Nonalcoholic steatohepatitis)治疗相关的专利**

**Case 4: CD137相关的生物药专利**



# Case 3: NASH(Nonalcoholic steatohepatitis)治疗相关的专利

Reaxys

Quick search Query builder Results Synthesis planner History

Search in: Reactions > Targets > Substances > Documents >

1,335 Documents with 92,242 Substances, 156,471 Reactions, 680 Targets

0 selected Limit To Exclude Export

NOVEL SPIROLACTONE COMPOUNDS

3, Wenjun - WO2019/6324, 2019, A1

es 60 Reactions 60 Targets Full Text >

Abstract hit: {...non-alcoholic steatohepatitis (NASH), acne, obesity, diabetes, and cancer. Also provided herein are pharmaceutical...}

Claims hit: {...non-alcoholic steatohepatitis (NASH).30. The method of claim 28 or 29, further comprising administering...}

3-HYDROXYBUTYRATE COMPOUNDS FOR USE IN REDUCING LIVER FAT

2 TDELTA LIMITED; CLARKE, Kieran - WO2019/2828, 2019, A1

Patent Family Members: GB201710229 D0; GB201810300 D0; WO2019/2828 A1

Abstract Claims Front Page Info Substances 3 Full Text >

Abstract hit: {...non-alcoholic steatohepatitis (NASH), alcoholic steatohepatitis (ASH) or non-alcoholic fatty liver (NAFL)...}

Claims hit: {...non-alcoholic steatohepatitis (NASH), alcoholic steatohepatitis (ASH) or non-alcoholic fatty liver (NAFL).13. A compound...}

COMPOSITIONS AND METHODS FOR TREATING OR PREVENTING ENDOCRINE FGF-LINKED DISEASES

3 YALE UNIVERSITY; SCHLESSINGER, Joseph; LEE, Sangwon - WO2019/10314, 2019, A1

Patent Family Members: WO2019/10314 A1

Abstract Claims Front Page Info Full Text >

Claims hit: {...(NAFLD), and nonalcoholic steatohepatitis (NASH).45. The method of claim 40, wherein the mammal...}

Filters

Limit to > Exclude >

Index Terms (List) >

Index Terms (ReaxysTree) >

Publication Year >

Document Type >

patent 1,335

Authors >

Patent Assignee >

Journal Title >

Substance Classes >

Reaction Classes >

Titles, Abstracts & >

Import Save Reset

CAS RN TI, AB & KW

ELSEVIER

COMPOSITIONS AND METHODS FOR TREATING OR PREVENTING ENDOCRINE FGF-LINKED DISEASES

2 YALE UNIVERSITY; SCHLESSINGER, Joseph; LEE, Sangwon - WO2019/10314, 2019, A1  
Patent Family Members: WO2019/10314 A1

治疗或预防内分泌fgf相关疾病的成分和方法

Abstract ^ Claims v Front Page Info ^ Full Text ↗

Abstract

The present invention relates in one aspect to the discovery that  $\beta$ -Klotho is the primary cell-surface receptor for FGF21, with FGFR1c functioning as a catalytic subunit that ultimately mediates intracellular signaling. In one aspect, the invention provides compositions and methods that are useful in treating or preventing endocrine FGF-related diseases or disorders.

Claims hit: {...(NAFLD), and nonalcoholic steatohepatitis (NASH).45. The method of claim 40, wherein the mammal...}

Front page info




发现有一部分文献与‘NASH’的治疗并没有关系

Assignees			Inventors (Authors)		
YALE UNIVERSITY; SCHLESSINGER, Joseph; LEE, Sangwon			SCHLESSINGER, Joseph; LEE, Sangwon		
Patent No	Kind Code	Publ. Date	Application No	Filing Date	Indexed Patent
WO2019/10314	A1	2019/01/10	WO2018-US40932	2018/07/05	yes
Priority No			Priority Date		
US2017-529215P			2017/07/06		
Patent Classification					
Main IPC		C07K 16/28			
Secondary IPC		G01N 33/50; G01N 33/574; G01N 33/68; G01N 33/74; A61K 39/395; A61K 45/06; A61P 3/04			






Search in: [Reactions >](#) [Targets >](#) [Substances >](#) [Documents >](#)

     
 Import Save Reset form Delete all

     
 Structure Molecular Formula CAS RN TI, AB & KW

Find search fields and forms

Reaxys 

◇ Titles, Abstracts & K... is ▼ NASH;"nonalcoholic steatohepatitis"  

AND

Group 3  Ungroup **IPC 分类辅助筛选适应症相关文献**   
 ◇ Patents: Main IPC is ▼ A61P 1/16  

AND  
 ◇ Patents: Secondary IPC is ▼ A61P 1/16

分类号	含义		
<a href="#">A</a>	农业		
<a href="#">A61</a>	医学或兽医学; 卫生学		
<a href="#">A61P</a>	化合物或药物制剂的特定治疗活性		
<a href="#">1/00</a>	治疗消化道或消化系统疾病的药物		
1/02	. 口腔用制剂, 例如治疗龋齿、口疮或牙周炎的药物		
1/04	. 治疗溃疡、胃炎或回流性食管炎的药物, 例如抗酸药、酸分泌抑制剂、黏膜保护剂		
1/06	. 镇痛药, 例如治疗结肠、食管痉挛性运动障碍的药物		
1/08	. 治疗恶心、晕动病或者眩晕的药物; 止吐药		
1/10	. 轻泻药		
1/12	. 止泻药		
1/14	. 助消化药, 例如酸类、酶类、食欲兴奋剂、抗消化不良药、滋补药、抗肠气胀药		
1/16	. 治疗肝脏或胆囊疾病的药物, 例如保肝药、利胆药、溶石药		
1/18	. 治疗胰腺疾病的药物, 例如胰酶		



# Case 4: 检索2019年2月，与CD137相关的，人用药，含抗原或抗体的医药配置品（生物药类专利）

The screenshot shows the Reaxys Query Builder interface. The search criteria are as follows:

- Group 1: Patents: Main IPC OR Patents: Secondary IPC, both containing 'a61k 39/00'.
- AND: Document Basic Index containing 'cd137'.
- AND: Patents: Date of publication containing '2019/02'.

Annotations on the screenshot:

- Contains 便于快速模糊检索**: Points to the 'contains' dropdown menu.
- 4个模块同时组合，并设定需要逻辑**: Points to the overall query structure with AND/OR operators.
- IPC分类:人用药类A61K, 含抗体类39/00**
- 关键索引: CD137**
- 公开日期: 2019年2月** (注: 该公开日期为专利的最后一个公开日期, 不一定是首发。可能是族号, 可能是不同版本的最新公开日期, 如, A1, A2, B)

# 组合模块构建

Reaxys

Quick search Query builder Results Synthesis planner History

Search in: Reactions > Targets > Substances > **关键词模块**

Import Save Reset form Delete all

Structure Molecular Formula CAS RN **Doc. Index**

在Query Builder中只需要点击所需模块即可进行组合检索

Drag & Drop to build a new query

查询特定模块

Find search fields and forms  
Q ipc

Reaxys ^

- ◇ Patents: Main IPC
- ◇ Patents: Secondary IPC

Feedback

# 检索结果

METHODS AND COMPOSITIONS FOR PREPARING GENETICALLY ENGINEERED CELLS

2 JUNO THERAPEUTICS, INC.; BONYHADI, Mark L. WO2019/32929, 2019, A1

Patent Family Members: WO2019/32929 A1

Abstract  Claims  **Front Page Info**  Full Text [↗](#)

Claims hit: {...of CD28, CD137 (4-1-BB), OX40, or ICOS.42. The method of claim 41, wherein...}

Assignees		Inventors (Authors)	
JUNO THERAPEUTICS, INC.; BONYHADI, Mark L.		BONYHADI, Mark L.	
Patent No	Kind Code	Publ. Date	Application No
WO2019/32929	A1	2019/02/14	WO2018-US46151
Priority No	公开日期 授权状况		Priority Date
US2017-543359P			2017/08/09
Patent Classification			
Main IPC	A61K 39/00		
Secondary IPC	C12N 5/0783		
<b>IPC 分类</b>			

## Claims

### CLAIMS

#### WHAT IS CLAIMED:

1. A method for genetically engineering (a) incubating an input composition, under stimulating conditions, a population of T cells, wherein the stimulating conditions comprise the presence of one or more intracellular signaling domains of one or more costimulatory molecules, thereby generating a stimulated cell composition, and (b) introducing a nucleic acid encoding a genetically engineered recombinant receptor, wherein the method thereby generates cells expressing the genetically engineered recombinant receptor.

2. A method for genetically engineering a population of T cells comprising naive-like T cells, wherein the stimulating conditions comprise the presence of one or more intracellular signaling domains of one or more costimulatory molecules, thereby generating a stimulated cell composition, and (b) introducing a nucleic acid encoding a genetically engineered recombinant receptor, wherein the method thereby generates cells expressing the genetically engineered recombinant receptor.

the incubating the input composition under stimulating conditions is performed prior to, during and/or subsequent to introducing a nucleic acid encoding a genetically engineered recombinant receptor.

3. The method of claim 1 or claim 2, wherein the incubating is carried out for at least 3 days.

4. The method of claim 1 or claim 2, wherein the incubating is carried out for at least 4 days.

5. The method of claim 1 or claim 2, wherein the incubating is carried out for at least 5 days.

6. The method of claim 1 or claim 2, wherein the incubating is carried out for at least 6 days.

7. A method for stimulating T cells, the method comprising:

(a) incubating, under stimulating conditions, an input composition comprising T cells comprising a culture-initiating amount of naive-like T cells or a CD8+ stimulated composition, wherein the stimulating conditions comprise the presence of a stimulatory reagent capable of activating one or more intracellular signaling components of a TCR complex and/or one or more intracellular signaling domains of one or more costimulatory molecules, thereby generating a stimulated cell composition, and (b) introducing into the stimulated cell composition a nucleic acid encoding a genetically engineered recombinant receptor, wherein the method thereby generates cells expressing the genetically engineered recombinant receptor.

(b) introducing into the stimulated cell composition a nucleic acid encoding a genetically engineered recombinant receptor, wherein the method thereby generates cells expressing the genetically engineered recombinant receptor.

专利‘Claim’部分的摘取和可索引，对于生物药类专利的检索非常有利。

通常生物药类的专利，不具有结构式，且专利标题和摘要一般会撰写得比较简单，造成了生物药类专利检索的困难



ELSEVIER



# Reaxys Medicinal Chemistry模块应用

## Case 5: 如何通过靶点筛选小分子抑制剂



# Case 5: 如何通过靶点筛选小分子抑制剂

Reaxys Quick search Query builder Results Synthesis planner History Peng Wu

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN

Find search fields and forms

Fields Forms History

Target Name is epidermal growth factor receptor binding protein;Epidermal growth factor receptor;epidermal growth factor-activated receptor

Substance Action on T... is inhibitor

Details information selection (highlighted)

Drug chemistry information search module (highlighted)

缩写快速转化相关靶点

is EGFR

- Targets 20,141,813
- protein 17,245,173
  - binding protein 3,108,588
    - protein binding protein 1,666,788
      - signaling receptor binding protein 67,023
        - growth factor receptor binding protein 271
          - epidermal growth factor receptor binding protein 7
- enzyme 9,455,640
  - catalytic acting on a protein 6,861,203
    - protein kinase 4,811,620
      - Protein kinase domain 3,631,410

Selected search items: epidermal gro... protein Epidermal gro...receptor epidermal gro... receptor EGFR EGFR (19del)

Clear selected Transfer

化合物作用效果

Su inhibitor

<input type="checkbox"/> activator	82,778
<input type="checkbox"/> agonist	849,420
<input type="checkbox"/> allosteric modulator	120,497
<input type="checkbox"/> antagonist	886,505
<input type="checkbox"/> blocker	156,879
<input type="checkbox"/> inactivator	2,044
<input checked="" type="checkbox"/> inhibitor	10,653,338
<input type="checkbox"/> inverse agonist	13,675
<input type="checkbox"/> irreversible antagonist	3
<input type="checkbox"/> irreversible inhibitor	83
<input type="checkbox"/> modulator	306,408
<input type="checkbox"/> opener	18,294
<input type="checkbox"/> partial agonist	707

1 of 2 Go to page

Clear selected Transfer



71.40 K

Filters

Limit to > Exclude >

By Structure

Measurement pX

Highest Clinical Phases

Targets

Parameters

Substance Classes

Molecular Weight

Number of Fragments

Availability

Availability in other databases

Available Data

Do

Pu

Patent Assignee

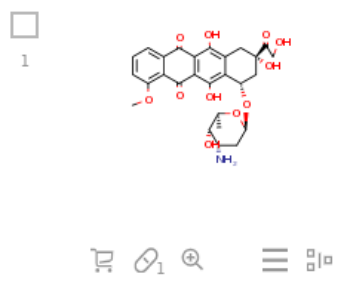
LogP

H Bond Donors

71,403 Substances out of 2,922 Documents, containing 102,517 Reactions, 375 Targets

0 selected

Sort by No of References



doxorubicin

C<sub>27</sub>H<sub>29</sub>NO<sub>11</sub> 543.527 1445814 23214-92-8

Identification

Druglikeness

Bioactivity (Hit Data)

Bioactivity (All)

Physical Data - 164

Spectra - 239

Other Data - 6,037

Preparations - 68 >

Reactions - 364 >

Targets - 393 >

Documents - 27,491 >

生物活性数据

doxorubicin

Identification

Druglikeness

Bioactivity (Hit Data)

Bioactivity (All)

Physical Data - 164

Spectra - 239

Bioactivity (All)

In vitro: Efficacy - 12410

In vivo: Animal Model - 2116

Metabolism - 756

Pharmacokinetic - 995

Toxicity/Safety Pharmacology - 12536

pX	Parameter	Value (qual)	Value (quant)	Unit	Action on target	Cell	Bioassay	Effect
14.9	IC50	=	1.3E-09	μM	Inhibitor	MMA cell line		
13.2	IC50		6.19E-08	μM		OVCAR-3 cell line	In Vitro (others)	antiproliferative agent
12.3	GI50	=	3E-07	μg/mL		NCI-H460 cell line		

建立构效关系

27,166 Substances out of 1,749 Documents, containing 57,983 Reactions, 222 Targets

0 selected Limit To Exclude Export Preparations

By Structure Measurement pX

Parameters

- ic50 27,166
- (no entry given) 25,029

Filter by value Substance Classes Molecular Weight Number of Fragments Availability Availability in other databases

doxorubicin C27H29NO11 543

Identification Druglikeness Bioactivity (Hit Data)

quercetol (HO)2C6H3C9H2O(

Identification Druglikeness Bioactivity (Hit Data)

Heatmap settings

数据 VS 化合物构效关系

Value of X-axis Parameter

Value of Y-axis Substances

Value of Cells Maximum of pX

Show substances  Names  Structure drawing

Display mode  Normal  Full Screen

Always show settings Apply >

Grid Heatmap

Preparations - 68 >  
Reactions - 364 >  
Targets - 393 >  
Documents - 27,491 >

Preparations - 180 >  
Reactions - 1,170 >  
Targets - 1,079 >  
Documents - 26,094 >

快速获取ic50数据



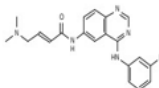
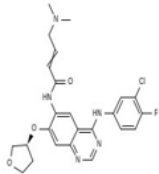
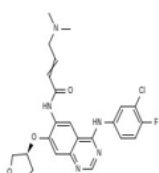
导出结果

ic50

Parameter

Substances

- staurosporine
- 4-[[3-chloro-4... nazoline
- 6,7-dimetho... -4-amine
- 4-Dimethyla... l]-amide
- (1R,5S)-3-(3-((...xan-1-ol
- N-(4-fluorop... -4-amine
- N-(3-chloro-... -4-amine
- N-(3-chloro-... -4-amine
- N-(3-chloro-... -4-amine
- N-(3-chloro-... -4-amine
- N-(3-chloro-... -4-amine
- N-(3-chloro-... -4-amine

A	B	C	D	E	F	G	H	I	J	K	L
Structure: Image	SMILES	CAS Registry Number	Chemical Name	Molecular Formula	Molecular Weight	Target Name	Target, Subunit, Species	Substance Action on Tar	Bioassay Category	Medchem: Measurement	Unit
	<chem>CN(C)CC=CC(=O)NC1=C2C=CC(=C2)C3=C1C(=O)N(C)C3</chem>		4-Dimethylamino-but-2	C20H20BrN5O	426.316	Epidermal growth factor	Epidermal growth factor Inhibitor		In Vitro (Efficacy)	IC50	nM
	<chem>CN(C)CC=CC(=O)NC1=C2C=CC(=C2)C3=C1C(=O)N(C)C3</chem>		4-[[3-chloro-4-fluorophenyl]piperidin-1-yl]piperidine	C24H25ClFN5O3	485.946	epidermal growth factor	epidermal growth factor Inhibitor		In Vitro (Efficacy)	IC50	nM
	<chem>CN(C)CC=CC(=O)NC1=C2C=CC(=C2)C3=C1C(=O)N(C)C3</chem>		4-[[3-chloro-4-fluorophenyl]piperidin-1-yl]piperidine	C24H25ClFN5O3	485.946	epidermal growth factor	epidermal growth factor Inhibitor		In Vitro (Efficacy)	IC50	nM



# RMC-特定的信息检索方法

◇ Target Name	⋮
◇ Substance Action on Target	⋮
◇ Substance Effect	⋮
◇ Measurement pX	⋮
◇ Target Nature	⋮
◇ Target Mutant/Chimera Details	⋮
◇ Target Transfection	⋮
◇ Substance RN	⋮
◇ Substance Route of Adm.	⋮
◇ Substance Dosing Regimen	⋮

◇ Biological Material Name	⋮
◇ Biological Species	⋮
◇ (Clinical) findings / disease	⋮
◇ Organs/Tissues	⋮
◇ Cells/Cell Lines	⋮
◇ Cell Fraction	⋮
◇ Measurement Parameter	⋮
◇ Measurement Qualitative	⋮
◇ Measurement Unit	⋮

### Substance Action on Target

Search

<input type="checkbox"/> activator	75,140
<input type="checkbox"/> agonist	1,929
<input type="checkbox"/> allosteric modulator	1,961
<input type="checkbox"/> antagonist	1,683
<input type="checkbox"/> blocker	160,460
<input type="checkbox"/> inactivator	1,996
<input type="checkbox"/> inhibitor	10,470,915
<input type="checkbox"/> inverse agonist	13,321
<input type="checkbox"/> irreversible antagonist	3
<input type="checkbox"/> irreversible inhibitor	83
<input type="checkbox"/> modulator	313,006

1 of 2    Go to page    Clear selected    Transfer

检索对靶点作用机制的特点信息时的模块

激动剂

阻断剂

抑制剂

### Measurement Parameter

is    Enter search term

> cellular parameters	94,814
> epidemiological data	120,359
> in-vitro pharmacological parameters	20,175,771
> in-vivo pharmacological parameters	46,741
> mathematical parameters	148,038
> medical parameters	32,006
> metabolic parameters	54,026
> metabolism/transport parameters	110,315
> microbiological parameters	286,015
> pharmacokinetic parameters	835,343
> absorption parameters	59,818
> F (drug bioavailability)	56,062
> kabs	1,550
> MAT (mean absorption time)	7
> t1/2 abs	589
> tlag	1,582

Transfer

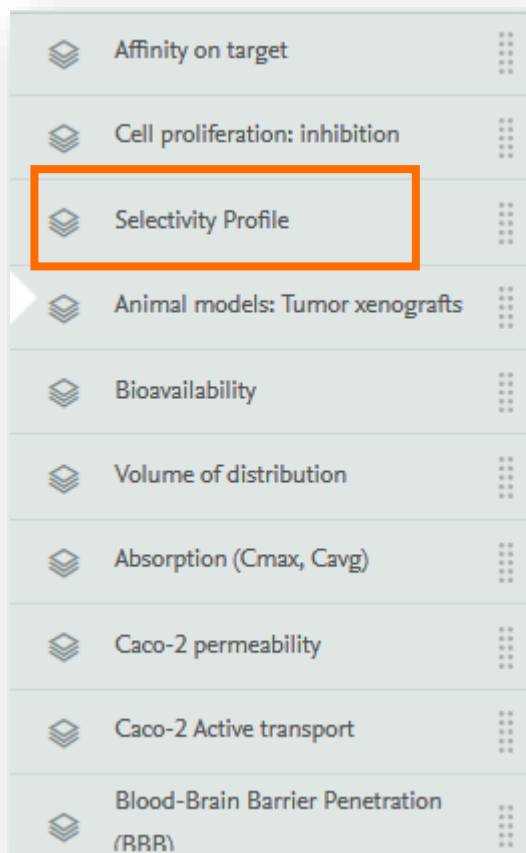
直接检索特定数据时的模块如PK的各种数据

各种分类细致的信息检索模块，快捷锁定对应结果



# RMC-组合信息便捷检索

预设的组合检索模块，便捷检索综合信息，如对于不同亚型的同类靶点，差异抑制性



**靶点选择性检索**

**靶点名称**

AND

抑制‘数量级’以‘mol’为单位换算，9=10的负9次方

COMBI

AND

Target Name	Operator	Value
Histone deacetylase 2	is	9
Histone deacetylase 8; Histone deacetylase [Neovison vison]; Histone deacet...	is	8



# RMC-组合信息便捷检索

- Affinity on target
- Cell proliferation: inhibition
- Selectivity Profile
- Animal models: Tumor xenografts
- Bioavailability
- Volume of distribution
- Absorption (Cmax, Cavg)
- Caco-2 permeability
- Caco-2 Active transport
- Blood-Brain Barrier Penetration (BBB)

- Cytotoxicity
- hERG inhibition
- Cytochrome inhibition (CYP3A4)
- Metabolism by cytochrome (CYP2D6)
- Microsomal stability
- Protein binding (blood, plasma)
- Cardiotoxicity

### hERG inhibition

- Structure  
Create Structure / Reaction Drawing
- AND
- Target Name  
is Target Name 'Potassium voltage-gated channel subfamily H mem'
- AND
- Target Nature  
is Target Nature 'wild'
- AND
- Measurement Parameter  
is Measurement Parameter '%50';'K';'Kd';'kd'
- AND
- Measurement pX  
Measurement pX

### Caco-2 permeability

- Structure  
Create Structure / Reaction Drawing
- AND
- Cells/Cell Lines  
is 'Caco-2 cell line';'Caco-2'
- AND
- Measurement Parameter  
is 'papp (a-b);'papp (b-a);'papp (transport)';'papp';'transport ratio';'transp'

只需要特定结构即可初步快速检索特殊信息

Thank you

