



ScienceDirect AI

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助力提升科研与知识发现效率

爱思唯尔·中国 刘万勇



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议程

- 新技术挑战下的AI变革
- 爱思唯尔对AI发展的思考与创新
- ScienceDirect AI提升科研与知识发现效率
- 关于爱思唯尔及未来展望

从现实角度来看，AI在
当今实际的科学研究领
域能起到什么作用？



传统的科研信息获取思路：以国产新冠药物的研发为例

35,491篇：2021年前新冠治疗药物相关文献

3,307 地塞米松

788 巴瑞替尼

4,616 托珠单抗

9,281 羟氯喹

5,753 瑞德西韦

4,993 阿奇霉素

884 伊维菌素

2260 法匹拉韦

5,753篇：瑞德西韦治疗新冠相关文献

257篇：瑞德西韦中间代谢物相关文献

172篇：GS-441524相关文献



ScienceDirect AI的实际使用：以国产新冠药物的研发为例

①背景调研

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2021年以前能有效治疗新冠的药物有哪些

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瑞德西韦的优势：
效果最明显且副作用低

- **Remdesivir**: Approved for severe COVID-19 cases due to its ability to inhibit viral RNA chain elongation (Tanimoto et al., 2022), (Wu et al., 2022), (Moriello et al., 2023).
- **Lopinavir/Ritonavir**: Initially studied but showed no significant benefit (Tan & Aboulhasan, 2020).
- **Favipiravir**: Approved in Thailand for COVID-19 treatment (Sirisubot et al., 2022).
- **Anti-inflammatory Agents**:
 - **Dexamethasone**: Used for patients with respiratory failure to reduce inflammation (Tanimoto et al., 2022).
 - **Tocilizumab**: An anti-IL-6 agent used for its potential clinical benefits (Lima-Morales et al., 2021), (Wahlström et al., 2024).
 - **Baricitinib**: Approved in Japan for its anti-inflammatory and antiviral effects (Tanimoto et al., 2022), (Wahlström et al., 2024).
- **Combination Therapies**:
 - **Interferon beta-1b, Lopinavir-Ritonavir, and Ribavirin**: Showed promising improvement (Lima-Morales et al., 2021).
 - **Hydroxychloroquine plus Azithromycin**: Used in combination therapy (Lima-Morales et al., 2021).

瑞德西韦的作用机制
依赖中间体抑制病毒！

- **Prodrug Conversion**: Remdesivir is a mono-phosphoramidite prodrug that is its active form, remdesivir-triphosphate (RDV-TP), an adenosine analog (Shen, Chavda & Mehta, 2023), (Hua et al., 2022), (Glen et al., 2023).
- **Inhibition of RdRp**: RDV-TP competes with adenosine-triphosphate for incorporation into the viral RNA chain. Once incorporated, it causes delayed chain termination, the synthesis and preventing the virus from replicating effectively (Shen, Chavda & Mehta, 2023), (Hua et al., 2022), (Glen et al., 2023).
- **Clinical Use and Efficacy**: Remdesivir has been approved by the U.S. FDA for treatment of severe COVID-19 cases. Clinical studies have shown that it can improve clinical recovery time in hospitalized patients (Shen, Chavda & Mehta, 2023), (Hua et al., 2022), (Glen et al., 2023).
- **Limitations and Recommendations**: Despite its antiviral activity, remdesivir's mortality and overall clinical outcomes remains modest. The WHO does not recommend its use due to insufficient evidence of significant benefits in survival (Hua et al., 2022), (Kawar et al., 2024), (Shah et al., 2023).

In summary, remdesivir works by inhibiting the viral RNA polymerase, thus block

②具体领域科研信息汇总

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瑞德西韦治疗新冠的机理是什么

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③科学原理总结

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瑞德西韦进入体内后会生成什么

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Summary answer
When remdesivir enters the body, it undergoes a series of metabolic transformations pharmacologically active. Here is a step-by-step breakdown of this process:

有效的中间体：
441524效果最好
易于合成且毒性低

- **Additional Metabolites**: Another significant metabolite formed is GS-441524, a predominant and persistent metabolite in human blood plasma (Zheng et al., 2022), (Bakhti et al., 2023), (Divya & Shabeer, 2024). GS-441524 is also noted for its activity against SARS-CoV-2 and has advantages such as easier synthesis and lower toxicity to remdesivir (Zheng et al., 2022).
- **Pharmacokinetics**: The active metabolite GS-443902 is found in high concentration, significantly above the effective concentration needed to inhibit SARS-CoV-2 (Divya & Shabeer, 2024). GS-441524 also accumulates over time, reaching a steady state of treatment (Divya & Shabeer, 2024).

④现存问题

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GS-441524治疗新冠的优缺点都有哪些

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Summary answer

Advantages of GS-441524 for Treating COVID-19:

- **Efficacy**: GS-441524, the parent nucleoside of remdesivir, has shown strong activity against SARS-CoV-2 in vitro and in vivo (Zheng et al., 2022), (Lei et al., 2022).
- **Oral Bioavailability**: GS-441524 has demonstrated favorable oral bioavailability studies, suggesting potential for oral administration, which is a significant advantage over remdesivir that requires intravenous administration (Lei et al., 2022), (Xie & Varghese, 2023).
- **Safety and Toxicity**: Preliminary clinical results indicate that orally administered GS-441524 is well-tolerated and shows promise for treatment (Zheng et al., 2022).

GS-441524的缺点：
口服生物利用度低

- **Oral Bioavailability Challenges**: Despite its favorable bioavailability, the oral administration of GS-441524 may still face challenges in achieving the necessary systemic exposure to be effective against SARS-CoV-2 (Wang, Yang & Song, 2023), (Cox et al., 2023).
- **Short Half-Life**: GS-441524 has a short in vivo half-life, which may limit its duration of action and require more frequent dosing (Zhou et al., 2023).
- **Potential Toxicity**: There is evidence suggesting that GS-441524 can cause renal toxicity, as observed in preclinical studies (Furusho et al., 2023).

In summary, while GS-441524 shows promise due to its efficacy, oral bioavailability and safety concerns remain challenges related to its use in clinical practice.

⑤潜在解决思路

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提高GS-441524的口服生物利用度

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Summary answer

Improving Oral Bioavailability of GS-441524

To enhance the oral bioavailability of GS-441524, several strategies have been explored:

- **Prodrug Development**:
 - **GS-421763**: This prodrug has shown high oral bioavailability in non-human primates and other relevant animal species. It efficiently converts to GS-441524 in the plasma and lungs, maintaining antiviral activity against SARS-CoV-2 and reducing viral load and lung pathology in a COVID-19 mouse model (Cox et al., 2023), (Xu et al., 2022).
 - **NCD 3 (obeldesivir)**: Another prodrug, NCD 3, has demonstrated improved oral bioavailability compared to GS-441524, delivering the bioactive metabolite effectively through oral administration. It is currently in Phase 3 clinical trials.

AI提到了异丁酸酯

- **Chemical Modifications**:
 - **Mono-isobutyric Acid Esters and L-valine Esters**: These compounds (So, Sb, Sc, Sd) have been synthesized to improve cellular permeability and exhibit stronger anti-SARS-CoV-2 activities than GS-441524 (Wei et al., 2023).
 - **5'-OH Simple Ester Prodrug**: This modification has significantly improved the oral absorption of GS-441524 (Zhou et al., 2023).
- **Formulation Techniques**:
 - **Microencapsulation**: Encapsulating GS-441524 in polymeric microspheres can protect it from degradation in the gastrointestinal tract and enhance its absorption (Zhou et al., 2023).
 - **Self-emulsifying Drug Delivery Systems (SEDDS)**: Formulating GS-441524 in SEDDS can improve its solubility and oral bioavailability (Zhou et al., 2023).

ScienceDirect AI的实际使用：以国产新冠药物的研发为例

⑥节点文献原文



⑦创新成果

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哪种酯的口服利用度高

Based on the information provided in the article, the ester prodrug with the highest oral bioavailability was the tri-isobutyrate prodrug 5g-HBr:

- The tri-isobutyrate prodrug 5g-HBr exhibited excellent oral bioavailability of 98.7% in mice.
- This was higher than the oral bioavailability of two mono-isobutyryl ester prodrugs: 5a (72.6%) and 5g (72.6%).

关键性成果：

异丁酸酯口服利用度高

Necessary to determine the optimal prodrug candidate among these high bioavailability prodrugs. However, based on the data presented, the tri-isobutyrate prodrug 5g-HBr appears to have the highest oral absorption in mice.



⑧潜在突破方向

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异丁酸酯的缺点有哪些

The article does not explicitly mention any major drawbacks or limitations of the isobutyryl ester prodrugs. However, it does provide some insights:

- Stability in simulated intestinal fluid (SIF):
 - The 3'-isobutyryl ester 5a showed good stability

缺点：

在体内不耐受,酯酶不稳定

Remaining after 4 hours in SIF: [1]

essential for first-pass metabolism:

Due to the high level of esterases in mouse plasma, the parent ester prodrugs were hardly detected, suggesting potential for first-pass metabolism. [2]

Need for further evaluation:

突破方向：

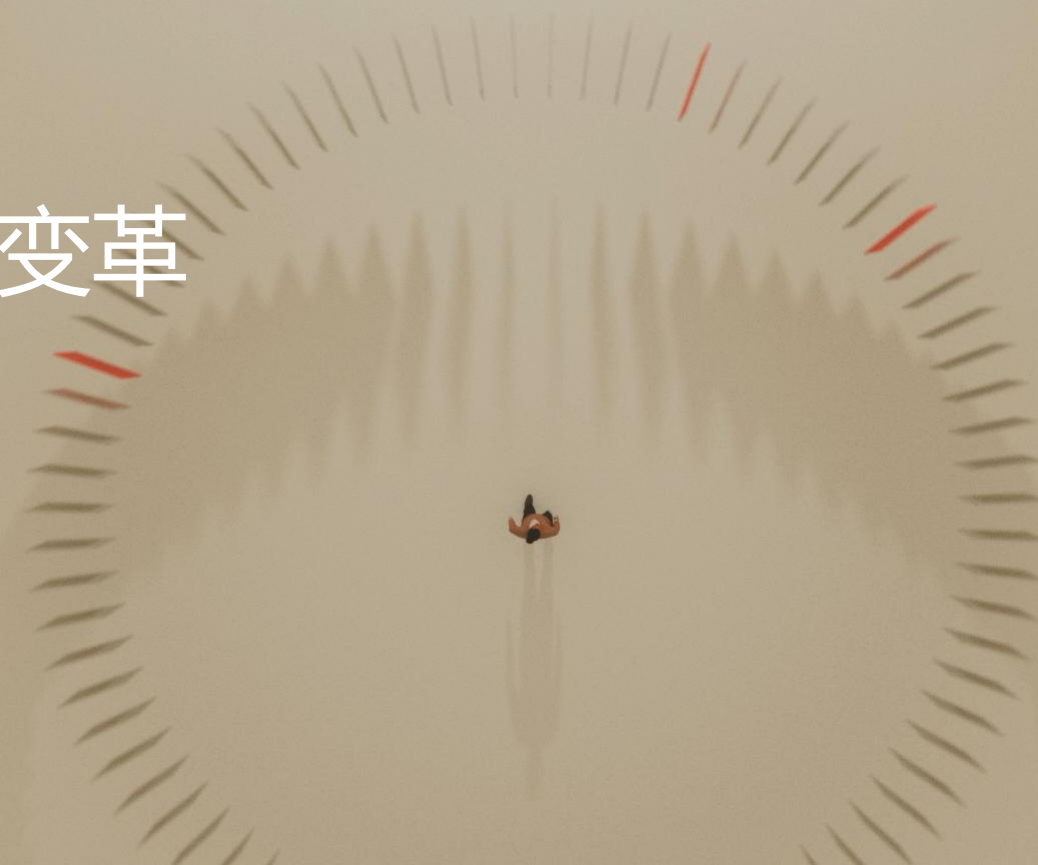
降低异丁酸酯的酶解活性
重复前面的科学问题可以得到氘代修饰可以解决相关问题



01

新技术挑战下的AI变革

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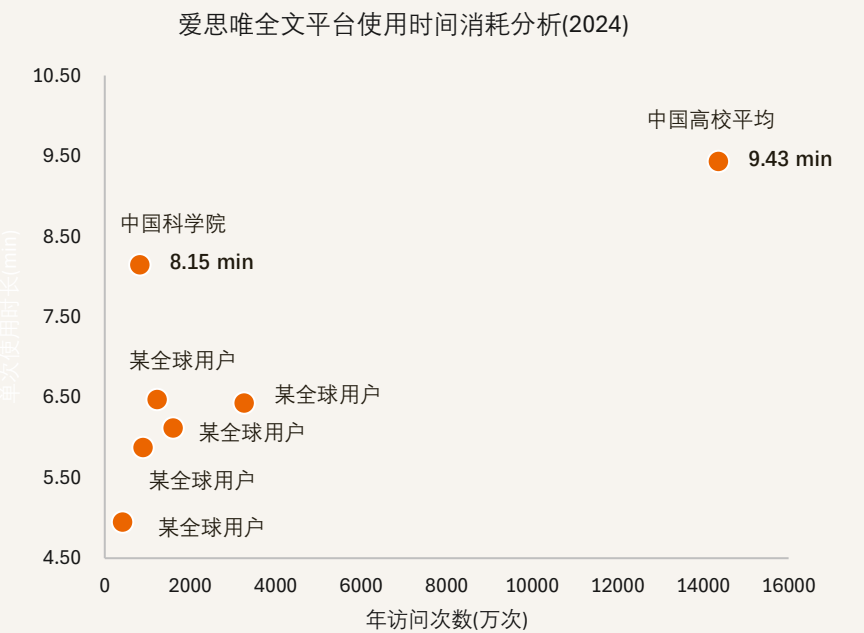


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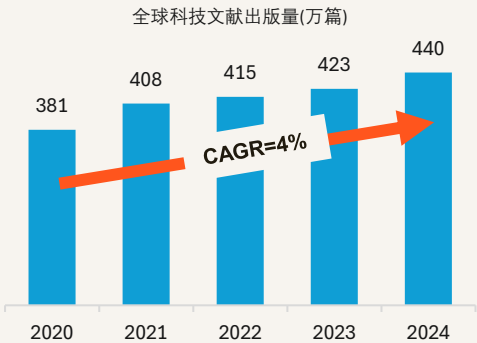
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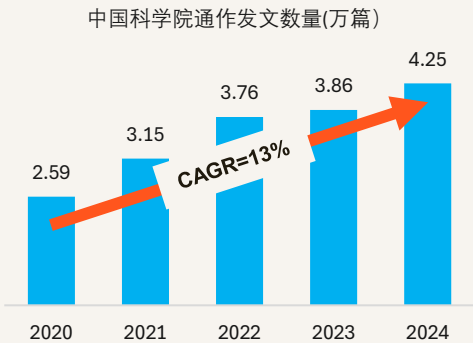


科研文献信息处理需求不断提升

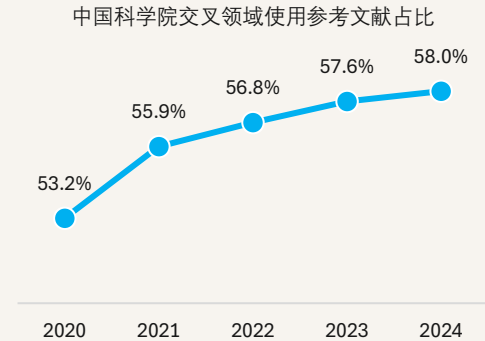
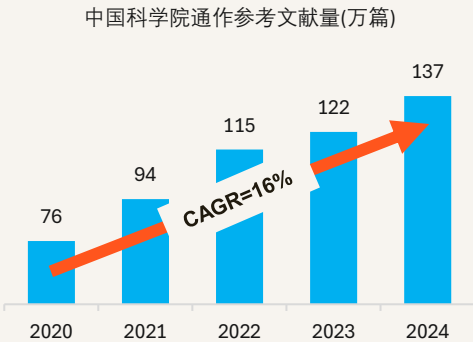
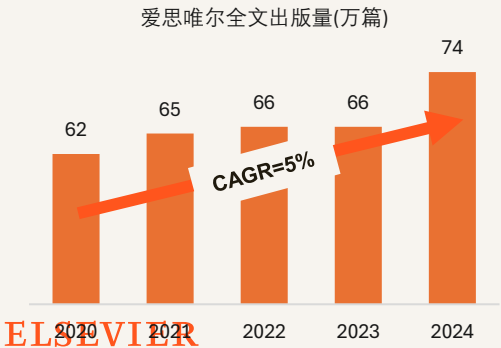
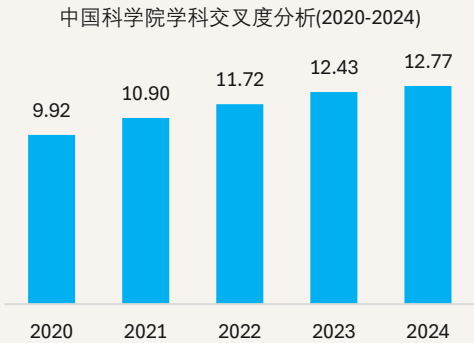
可获取的科研信息增长迅猛



中国科学院科研产出不断上涨



跨学科研究不断积累



科研人员检索证据花费的时间？

- 发表文章数量与长度快速增长。信息过载，检索困难
- 76%的科研人员使用AI辅助阅读
- 多数AI工具仅为概率性词汇预测，输出错误且无法追溯的答案，现有AI工具无法分析全文
- 图书馆对非科研AI工具表示担忧

阅读占据了科研人员大部分时间

35%

的时间



每周14小时

确保AI基于**高质量、可信赖的内容**，并且具备**足够的透明度**，是科研人员和临床医生眼中AI应用于其工作的前提条件。

传统科学研究模式的局限性以及AI带来的科研范式变革

传统科研的局限性



文献过载

- 个人阅读范围限制
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线性思维局限

- 实验室条件、专业背景、人员限制
- 难以实现跨领域突破



经验依赖

- 前沿探索高度依赖小范围内的积累
- 问题解决的路径依赖



试错成本高

- 科研周期长
- 纠偏依赖非即时反馈

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AI的应用促进了科研范式变革



知识获取革命:

- 领域脉络生成
- 跨学科知识图谱构建
- 核心问题聚焦



效率提升:

- 文献调研
- 实验设计与数据分析
- 论文发表



创新模式转变:

- 科研洞察力加强
- 跨学科方法迁移
- 实时动态纠偏

Source: Artificial intelligence in systematic reviews: promising when appropriately used

现成AI解决方案在科学研究场景中的不足

数据基础

非同行评议内容
非全文内容
学科覆盖度不足

训练模型目标

模型训练非科学研究

应用场景

局限于文献检索
文献精读涉及不多
较少提供实验对比

网络访问

不向我国提供服务
无法正常访问



科研流程的复杂性带来的挑战



选择
发表平台

如何
获取资金

寻找
合作者

从现有研究
中提取洞见

比较洞见

设计实验

开展实验

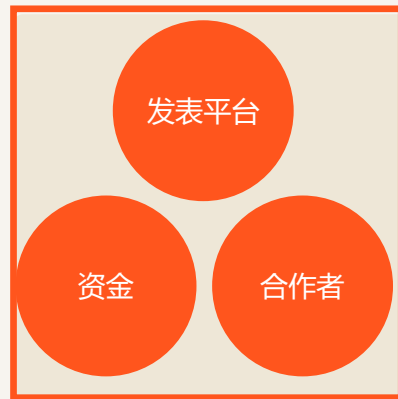
写作与发表

分享
研究成果

AI工具的应用有助于简化科研复杂性



战略与规划



Scopus AI的核心关注

阅读、分析与设计



ScienceDirect AI的核心关注

交付与分享



爱思唯尔对AI发展的思考与创新



爱思唯尔AI发展基石

坚持可靠的数据基础

- 基于同行评审的高质量科研成果

- 2100 万篇论文与图书章节
- 一亿条文献记录
- 3.29亿物质与0.69亿反应数据

坚持技术的可靠性

- 确保隐私与安全
- 规避AI幻觉
- 信息溯源

- 严格的大型语言模型提示工程设计
- AI生成结果始终引用源文本

坚持面向服务科学研究

- 持续的更新迭代
- 吸纳用户意见与反馈

- 与科学界140年的紧密合作
- 坚持用户至上
- 坚守爱思唯尔人工智能原则

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ScienceDirect® AI

功能的全面性

为科学研究全流程提供高效服务

广泛的参与性

全球70 个机构的 3 万多名研究人员参与测试

可靠性

所有结果均严格追溯至全文内容
专家审核制 & 严格规避AI幻觉

责任性

GPT 4o、4o-mini以及Claude 3.0 Haiku模型综合运用
严格遵守爱思唯尔AI原则

数据基础

经过同行评审的爱思唯尔高质量全文内容
涵盖所有学科1400万篇期刊与图书章节内容

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提升科研与知识发现效率

ScienceDirect AI四大核心功能



智能检索



实验对比



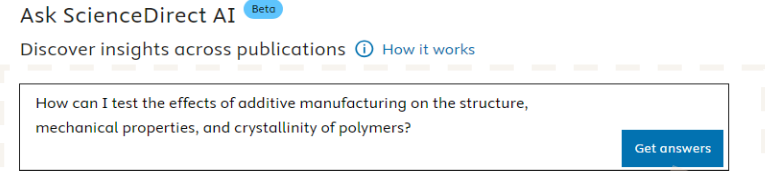
阅读助手



文献管理

智能检索，助力科研人员快速掌握前沿科技信息

利用全文数据生成专业的AI总结，帮助您用自然语言描述问题，从超过1400万篇文章和书籍章节中获取见解



Summary answer

Testing the Effects of Additive Manufacturing on Polymers

To test the effects of additive manufacturing on the structure, mechanical properties, and crystallinity of polymers, consider the following steps:

**1. Printing Parameters:

- **Crystallinity Variability:** Adjusting printing parameters can significantly affect the crystallinity within the polymer part, which in turn influences mechanical performance and chemical stability (Lee et al., 2022), (Hart, Dunn & Wetzel, 2020).
- **Thermal Cycles:** The complex thermal cycles during additive manufacturing can alter microstructures, impacting mechanical properties such as tensile strength (Lia et al., 2018).

**2. Mechanical Properties:

- **Internal Defects:** Monitor for internal defects like voids, which can affect mechanical properties and lead to failure in lattice structures under stress (Wei et al., 2024).
- **Print Orientation:** Investigate the effects of print orientation on mechanical properties. For instance, layer orientation can affect tensile fracture behavior and anisotropic mechanical performance (Palma et al., 2019), (Dai et al., 2024).
- **Process Parameters:** Vary process parameters such as infill pattern and density to observe changes in tensile, compression, flexural, or impact strength (Vallejos Baier et al., 2021).

节约80%
信息筛选时间

节约50%
文献阅读时间

- ① | 研究领域总结
- ② | 研究空白介绍
- ③ | 研究方法汇总
- ④ | 持续深入洞察
- ⑤ | 衍生问题推荐

对比实验：临床试验和其他实验比较

专注于每篇文章的核心部分，详细总结文献的实验方法、结果和结论，并对多篇相关文献进行比较



实验目标



实验条件



实验方法



实验结果



讨论总结

ARTICLE	EXPERIMENT / STUDY	GOAL	MATERIALS	METHODS	RESULTS	CONCLUSION
Article Increased fracture toughness of additively manufactured semi-crystalline thermoplastics via thermal annealing Kevin R. Hart, Ryan M. Dunn, Eric D. Wetzel <i>Polymer</i> • Volume 211 • 2020 Export article as CSV	Fracture toughness testing	To evaluate the critical elastic-plastic strain energy release rate (JIC) of the interlaminar region of additively manufactured single edge notched bend (SENB) specimens made from polylactide (PLA) polymer, and to study the effect of post-print thermal annealing and cooling rate on the degree of crystallinity and fracture toughness.	Single edge notched bend (SENB) specimens measuring 100 x 20 x 10 mm, fabricated using fused-filament fabrication (FFF) with 1.75 mm polylactide (PLA) filament, printer nozzle diameter of 0.5 mm, nozzle temperature of 200 °C, bed temperature of 50 °C, 454 layers with [0/90] orientation, 2 perimeter shells, 100% infill density, layer height of 0.22 mm, 12.7 µm thick poly-imide (Kapton) tape as pre-crack notch.	SENB specimens were subjected to post-print thermal annealing at 160 °C for 2 hours, then cooled at various rates (quenched in ice water or cooled at 1 °C/min) to induce different degrees of crystallinity. Fracture testing was performed in three-point bending in displacement control at 0.5 mm/min, with crack propagation monitored using a CCD camera. Fracture surfaces were analyzed using optical and scanning electron microscopy.	As-printed PLA SENB specimens had an interlaminar fracture toughness of 2.73 ± 0.48 kJ/m ² . Annealed and quenched specimens (amorphous, 0% crystallinity) had a toughness of 5.62 ± 1.81 kJ/m ² . Annealed and slowly-cooled specimens (25% crystallinity) had a toughness of only 0.63 ± 0.017 kJ/m ² .	Annealing can increase the interlaminar toughness of additively manufactured PLA, but only if the material is quenched rapidly after annealing to maintain an amorphous state. Slow cooling after annealing results in high crystallinity and low fracture toughness.
	Differential scanning calorimetry (DSC)	To determine the maximum enthalpy of cold crystallization (ΔH_{cc}^*) of PLA polymer, which establishes an upper limit on the degree of crystallinity that can be induced using common heating and cooling mechanisms.	PLA filament (1.75 mm diameter) pelletized by manually cutting into 10 mm segments, fed into a twin-screw micro-compounding machine at 200 °C and 50 rpm for 10 minutes to create an amorphous melt, then quenched in an ice water bath.	The quenched amorphous PLA extrudate was dried and then subjected to a heat-cool-heat DSC cycle between 40-200 °C at 5 °C/min to measure the maximum enthalpy of cold crystallization.	The maximum enthalpy of cold crystallization (ΔH_{cc}^*) for the fully amorphous PLA polymer was 21.7 J/g.	The maximum enthalpy of cold crystallization establishes an upper limit on the degree of crystallinity that can be induced in the PLA polymer using common heating and cooling mechanisms.

阅读助手：深度高效获取文献细节

节省阅读时间，针对**单一文章**回答用户提出的问题，提供详细解释和定制摘要，让您更高效地理解和利用文献的内容

全文快速总结：

1

创新点精确分析：

2

研究方法概要：

3

潜在突破方向：

4

View PDF Download full issue

Bioorganic & Medicinal Chemistry
Volume 46, 15 September 2021, 116364

Potency and pharmacokinetics of GS-441524 derivatives against SARS-CoV-2

Dailiao Wei^{a,d}, Tianwen Hu^{a,d}, Yumin Zhang^c, Wei Zheng^{b,d}, Haitao Xue^b, Yuanchao Xie^b, Hagi A. Aiso^{a,d}

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<https://doi.org/10.1016/j.bmc.2021.116364>

Abstract

The nucleoside metabolite of remdesivir, GS-441524 displays potent efficacy, and is being evaluated in clinical as an oral antiviral therapy. However, this nucleoside has a poor oral bioavailability in non-human. Herein, we reported a variety of GS-441524 derivatives with modifications on the base or the sugar moiety, as well as some including five isobutyryl esters, two L-valine esters, and one carbamate nucleosides, only the 7-fluoro analog **3c** had moderate anti-SARS-CoV-2 activity. The phosphoramidate prodrug **7** exhibited reduced activity in Vero E6 cells. The prodrugs, the 3'-isobutyryl ester **5a**, the 5'-isobutyryl ester **5c**, and the ester **5g** hydrobromide showed excellent oral bioavailabilities (F~71% respectively) in mice, which provided good insight into the pharmacokinetic optimization of GS-441524.

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Questions you could ask:

- What antiviral activity was observed in the synthesized GS-441524 derivatives against Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2)?
- What dosage of GS-441524 was found to suppress Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) replication in vivo?
- Which medication has received FDA approval for treating Coronavirus Disease 2019 (COVID-19) patients?

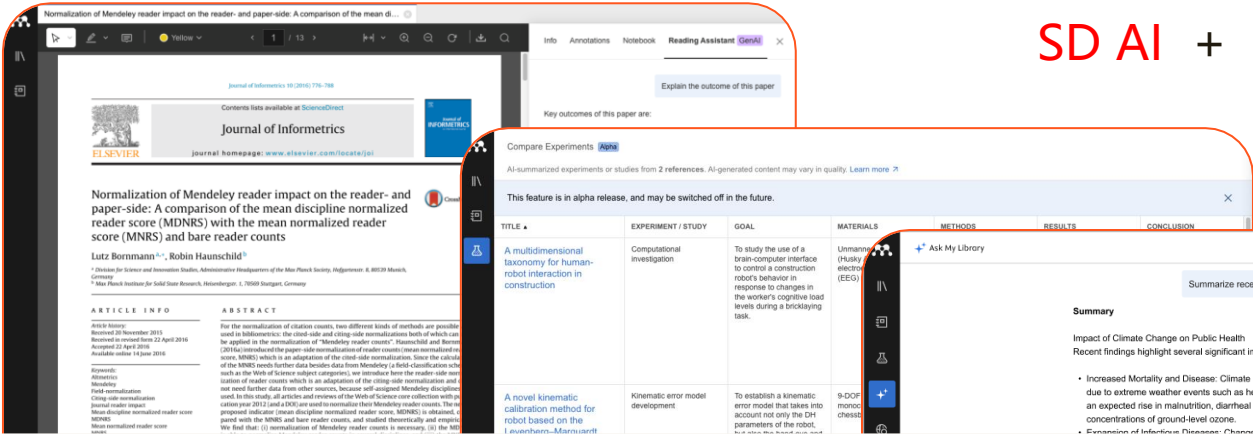
Actions you could take:

- Summarize this article
- Summarize experiments

Ask about this article

文献管理：跨平台赋能个性化科研洞察

SD AI +  Mendeley



The screenshot displays the ScienceDirect AI interface. On the left, a paper titled "Normalization of Mendeley reader impact on the reader- and paper-side: A comparison of the mean discipline normalized reader score (MDNRS) with the mean normalized reader score (MNRs) and bare reader counts" by Lutz Bornmann and Robin Haunschild is shown. The right panel features a "Compare Experiments" table with columns for Title, Experiment / Study, Goal, Materials, Methods, Results, and Conclusion. The table lists two experiments: a multidimensional taxonomy for human-robot interaction and a novel kinematic calibration method for robot-based systems. Below the table, a "Summary" section discusses the impact of climate change on public health, highlighting increased mortality and disease, and the expansion of infectious diseases.

TITLE	EXPERIMENT / STUDY	GOAL	MATERIALS	METHODS	RESULTS	CONCLUSION
A multidimensional taxonomy for human-robot interaction in construction	Computational investigation	To study the use of a brain-computer interface to control a construction robot's behavior in response to changes in the worker's cognitive load levels during a bricklaying task.	Umanini (Heavy electroencephalogram (EEG))			
A novel kinematic calibration method for robot based on the jacobian matrix	Kinematic error model development	To establish a kinematic error model that takes into account not only the DH parameters of the robot.	9-DOP motion chain			

Summary

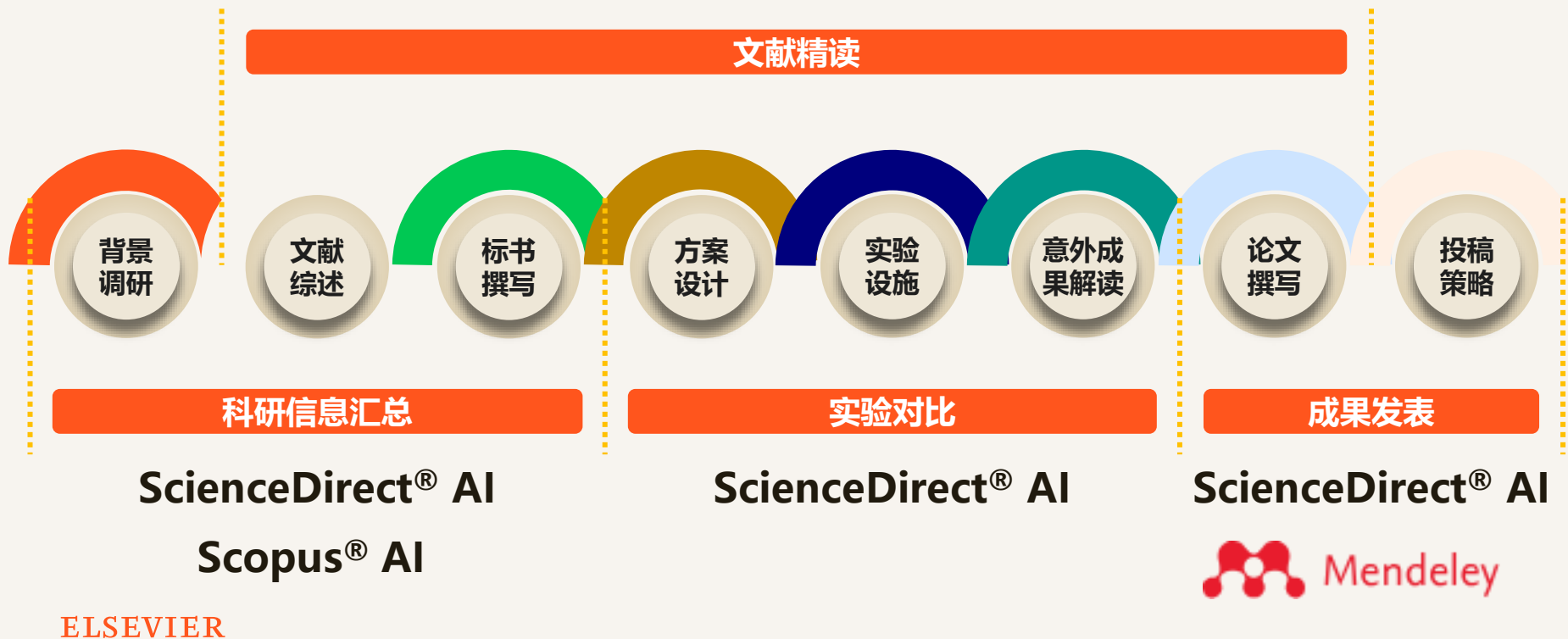
Impact of Climate Change on Public Health

Recent findings highlight several significant impacts of climate change on public health:

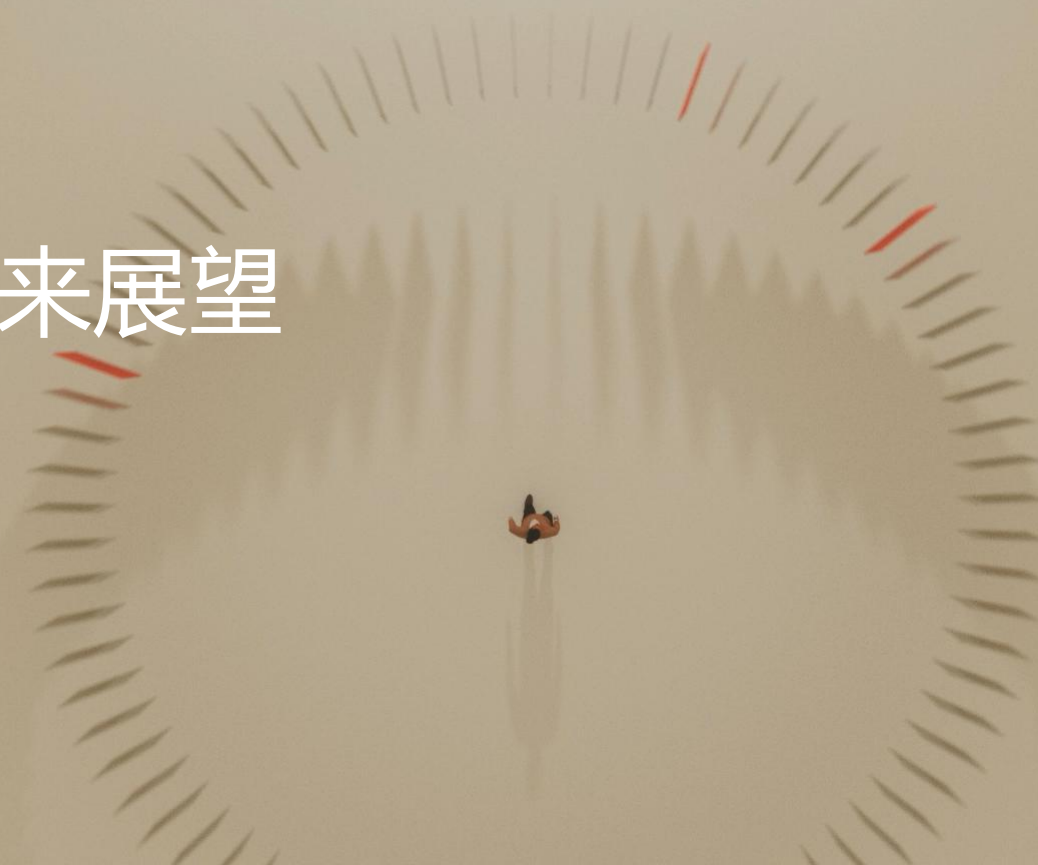
- Increased Mortality and Disease: Climate change is projected to increase deaths, diseases, and injuries due to extreme weather events such as heat waves, floods, storms, fires, and droughts. There is also an expected rise in malnutrition, diarrheal diseases, and cardio-respiratory diseases due to higher concentrations of ground-level ozone.
- Expansion of Infectious Diseases: Changes in climate are likely to alter the spatial distribution of

ScienceDirect AI用户可免费使用Mendeley AI功能，将文献分析从ScienceDirect平台延伸至个人，跨出版商文献库，真正实现“个性化检索、智能分析”，为个人科研的定制化深度分析和效率提升注入全新动能。

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- 人工智能
- 清洁能源

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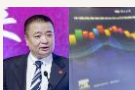
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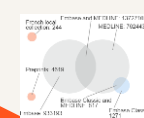
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