人工智能与天然药物动态监测快报

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政策与规划

EMA 发布 AI 在药品生命周期中使用的思考性文件

欧洲药品管理局（EMA）于 7 月 19 日发布了一份新思考性文件介绍了在整个产品生命周期和基于风险的背景下使用人工智能/机器学习（AI/ML）来开发和生产药物。思考性文件提供了有关 AI/ML 何时可用于开发产品以及如何在上市后环境中使用此类技术的见解。

该思考性文件由 EMA 大数据指导小组（BDSG）和药品监管机构负责人组织（HMA）联合编写。EMA 数据分析和方法主管、BDSG 联合主席 Peter Arlett 表示，“通过这篇文件，我们将与开发人员、学者和其它监管机构展开对话、讨论前进的方向，确保充分发挥 AI/ML 创新的潜力，造福患者和动物健康。”

EMA 表示，文件的目的是考虑在整个药品生命周期中使用 AI/ML，包括产品开发、许可和许可后阶段。鉴于 AI/ML 领域的快速发展，EMA 的目标是在使用此类新兴技术支持新产品开发时反思与监管审评相关的科学原理。

文件指出，“确定属于 EMA 或成员国国家主管当局职权范围的 AI/ML 方面至关重要，因为审评期间对数据的审查程度将取决于这一职权范围。这篇思考性文件仅关注 AI 在医药产品生命周期中的使用，任何对药物开发、相互作用等新方法的资格引用都应在这个范围内理解。”

但文件也指出，“采用 AI/ML 的医疗器械可以在临床试验的背景下使用，以生成支持上市许可申请的证据或可以与医药产品的使用相结合。在这种情况下，EMA 将参与评价该类器械的特性是否足以生成证据，支持欧盟上市许可。同样，如果器械用于在产品特性概要中提供建议，例如在计量学或监测方面，EMA 将评价拟议组合使用的所有相关方面。”

EMA 指出，AI/ML 工具有可能支持医药产品整个生命周期中数据的获取、转换、分析和解释。例如，EMA 表示，AI/ML 建模可用于替代、减少和完善临床前开发过程中动物模型的使用。在临床试验中，AI/ML 可能会支持根据某些疾病特征或其它临床参数选择患者。监管机构还表示，AI/ML 具有支持数据记录和分析的潜力，监管机构可以利用其这方面的潜力做出上市许可的决策。

EMA 表示，“在上市许可阶段，AI 的应用包括起草、编译、翻译或审查药物产品信息中数据的工具。在上市许可后阶段，此类工具可以有效支持药物警戒活动，包括不良事件报告管理和信号检测。”

EMA 补充指出，“这一系列应用带来了挑战，例如对算法的理解，尤其是对其设计和可能的偏差的理解，以及技术故障的风险和对 AI 在医药开发和卫生领域的应用产生的更广泛的影响。”

为应对这些挑战，思考性文件强调，以人为本的方法应该指导 AI/ML 技术的所有开发和部署。并且在药品生命周期中使用此类技术应始终遵守现有法律要求，考虑道德并确保对基本权利的恰当尊重。

如果 AI/ML 技术用于医药产品开发、评估或监测，并且预计会对产品的获益风险评价产生影响，那么产品开发人员应尽早征求监管机构的意见。

思考性文件指出，“有关风险管理的建议将进一步反映在未来的监管指南中，因为系统故障或模型性能下降的影响可能从很小到严重，甚至危及生命。风险程度可能不仅取决于 AI 技术，还取决于 AI 技术的使用背景和影响程度。此外，风险程度可能会在 AI 系统的整个生命周期中有所不同。计划部署 AI/ML 的上市许可申请人或上市许可持有人（MAH）应考虑并系统地管理从早期开发到退出使用的相关风险。”

HMA/EMA 计划于 2023 年 11 月 20 日至 21 日举行研讨会，讨论该思考性文件草案。利益相关者可以在 12 月 31 日之前对文件反馈意见。

信息来源：https://new.qq.com/rain/a/20230724A09JCJ00

项目计划

加速新药问世，欧洲更新“优先药物计划”

4 月 4 日，欧洲药品管理局（EMA）宣布，其正在向优先药物（PRIME）计划引入一些新功能，以加强对那些处于医疗需求高度未竟领域药物开发的支持。PRIME 计划使患者能够更早获得改变生活的药物。截至 2022 年底，共有 26 种受到 PRIME 支持的药物获得了欧盟（EU）批准的积极推荐。

为了优化对有前景药物的早期科学和监管支持，EMA 将为每个 PRIME 开发项目建立一份发展蓝图以及产品开发跟踪系统。这两个工具将便于在整个药物开发过程中监测开发进度并确定需要进一步讨论的关键议题，从而促进监管机构与药物开发者之间的持续对话。

此次的“新功能”项目是一项自 2023 年 3 月开始、为期 12 个月的试点项目。如相关的 PRIME 开发项目在已获得全面初步建议后遇到具体问题，现在可以为这些项目提供快速的科学建议。这种灵活的科学建议设置将使得 EMA 在更短的时间内解决来自 PRIME 申请者的疑问。

最后一个新功能是提交准备会议，该会议将在向 PRIME 药物开发者提交上市许可申请前约一年举行。这些会议的目的是讨论药物开发状态，包括先前监管建议的实施情况以及拟支持上市许可申请的数据包。潜在申请者还将需要提供成熟的上市后证据生成计划（如适用）。

上述所有举措旨在促进并加速为上市许可申请的评估产生健全且相关的证据，这将使患者能够更早地获得可以带来真正改变的变革性治疗。

信息来源： https://www.163.com/dy/article/I2GR8KTU05349C3E.html

基金委发布“RNA 病毒性传染病广谱治疗药物创新基础研究”重大项目指南

2023-05-30

国家自然科学基金委员会于 5 月 30 日发布“RNA 病毒性传染病广谱治疗药物创新基础研究”重大项目指南。项目目标是：基于 RNA 病毒感染与致病的共性机制，针对药物新靶点、新理论、新策略与新方法等，开展系统、创新的基础研究，设计并发现广谱适用、活性明确、安全性好、成药率高的原创抗病毒候选药物并阐明作用机制，为我国自主研发 RNA 病毒性传染病原创治疗药物提供基础支撑。

申请书提交时间为 2023 年 8 月 25 日至 8 月 31 日 16 时。

详见国家自然科学基金委员会网站。

信息来源: https://www.nsfc.gov.cn/publish/portal0/tab434/info89426.htm

研究前沿

颠覆基因研究和药物开发，AI 绘制基因互作网络，加快疾病治疗靶点发现

2023-07-03

近日，美国丹娜-法伯癌症研究所的研究人员在 Nature 期刊发表了题为：Transferlearning enables predictions in network biology（迁移学习使网络生物学的预测成为可能）的研究论文。

这项研究生成了一个基因表达数据集——Genecorpus-30M，其中包括来自各种人体组织的约 3000 万个单细胞转录组数据。研究团队通过使用该数据集预训练了一个基于迁移学习的 AI 模型——Geneformer，以实现在有限的数据下预测基因网络动力学、绘制基因网络图谱、加快发现疾病治疗候选靶点。

在这项最新研究中，研究团队试图开发和预训练一个具有大型通用基因表达数据集的深度学习模型，以便它可以“理解”基因网络动力学，并且可以在缺乏数据的情况下在广泛的应用中提供有关基因相互作用和细胞状态的预测。

为了达到这个目的，研究团队首先利用公开的数据生成了一个基因表达数据集——Genecorpus-30M，其中包括来自广泛的人体组织的大约 3000 万个单细胞转录组数据。然后，研究团队使用该数据集预训练基于迁移学习开发的深度学习模型——Geneformer，以实现对基因网络动力学的基本预测。

研究团队发现，当 Geneformer 针对与基因网络动态或 DNA-蛋白质复合物染色质修饰相关的各种任务进行修饰时，与标准替代方法相比，它始终提高了预测准确性。

在这项研究中，当使用有限的特定于心肌疾病的基因表达数据进行微调时，Geneformer 确定了候选的治疗靶点。在基于诱导多能干细胞（iPSC）的心肌疾病模型中靶向这两种候选细胞，能够导致由 iPSCl 再分化的心肌细胞收缩功能改善。

总而言之，这项研究基于迁移学习开发了一个可以绘制基因网络的深度学习模型——Geneformer，通过预训练、微调和转移其对基因网络动力学的“理解”，Geneformer 可以应用于广泛的研究领域，在有限的数据中加速发现关键的网络调控因子和候选治疗靶点。

信息来源：https://new.qq.com/rain/a/20230703A03DON00

推荐评论：

*利用有限的数据提取关键信息加速候选靶点发现愈来愈重要。

*机器学习和生物学的交叉研究，为理解“微观复杂的生命过程”开辟了强大有力的途径，有望为疾病治疗提供一种高效的候选靶点鉴定方法。

华大智造研发团队训练自博弈 AI 智能体，实现高效蛋白质从头设计

2023-07-21

2023 年 7 月 20 日，华大智造杨梦团队在 Nature 子刊 Nature Machine Intelligence 上发表了题为：Self-play reinforcementlearning guides protein engineering 的研究论文，发布了一款名为“EvoPlay”的强化学习算法模型。

EvoPlay 借鉴围棋自博弈（Self-play）的方式搜索海量蛋白质突变空间，并通过结合不同的功能或结构预测模拟器，像自动驾驶一样训练一个智能体（Agent）完成指定功能增强的蛋白进化。研究团队将 AlphaFold 家族模型和 AlphaGo 家族模型有机结合，从而以折叠结构为目标高效地设计蛋白质。

值得一提的是，蛋白质的工程化设计和改造是基因测序仪的底层基础，基因测序仪的迭代升级离不开蛋白工程技术的突破。科学家们通过改造各种各样的蛋白质操纵 DNA 分子、读取酶催化的信号从而识别碱基序列。从华大智造测序仪试剂里用到的聚合酶、荧光素酶等各种工具酶，到更广范围的生物催化剂、生物传感器、治疗类抗体到生物燃料，都离不开对蛋白质的设计和改造。。

信息来源：https://new.qq.com/rain/a/20230721A001QL00

推荐评论：

蛋白质是重要的生物大分子，其本身可作为药物、催化剂等参与众多生命活动过程。AI 赋能的蛋白质从头设计将加速相关蛋白质药物、生物催化剂的研究与开发，进而促进相关领域的研究及产业发展。

Meldrum-Based-1H-1,2,3-三唑类抗糖尿病药物的合成、体外 α-葡萄糖苷酶抑制活性、分子对接研究和计算机实验方法

A series of novel alkyl derivatives (2–5a,b) and 1H-1,2,3-triazole analogues (7a–k) of Meldrum’s acid were synthesized in a highly effective way by using “click” chemistry and screened for in vitro α-glucosidase inhibitory activity to examine their antidiabetic potential. 1H NMR, 13C-NMR, and high-resolution electrospray

ionization mass spectra (HR-ESI-MS) were used to analyze each of the newly synthesized compounds. Interestingly, these compounds demonstrated high to moderate α-glucosidase inhibitory potency having an IC50 range of 4.63–80.21 μM. Among these derivatives, compound 7i showed extraordinary inhibitory activity and was discovered to be several times more potent than the parent compound Meldrum (1) and the standard drug acarbose. Later, molecular docking was performed to understand the binding mode and the binding strength of all the compounds with the target enzyme, which revealed that all compounds are well fitted in the active site of α-glucosidase. To further ascertain the structure of compounds, suitable X-ray single crystals of compounds 5a, 7a, and 7h were developed and studied. The current investigation has shown that combining 1H-1,2,3-triazole with the Meldrum moiety is beneficial. Furthermore, this is the first time that the aforementioned activity of these compounds has been reported.

信息来源：Satya Kumar Avula, Saeed Ullah, Sobia Ahsan Halim, Ajmal Khan, Muhammad U. Anwar, René Csuk, Ahmed Al-Harrasi, and Ali Rostami

ACS Omega 2023 8 (28), 24901-24911

https://pubs.acs.org/doi/10.1021/acsomega.3c01291

推荐评论：

*运用 MS/MS 数据库挖掘具有特定结构特征的工具较为重要。

*机器学习和生物学的交叉研究，为理解“微观复杂的生命过程”开辟了强大有力的途径，有望为疾病治疗提供一种高效的候选靶点鉴定方法。

*该研究呈现了一种基于二级质谱定向挖掘具有特定特征的天然产物的新方法，对于天然产物化学研究，尤其是针对特定类型天然产物的研究具有潜在价值。

通过基于结构的虚拟筛选、动力学模拟和 DFT 研究鉴定 Mulberrofuran 作为甲型肝炎病毒 3C（pro）和 RdRP 酶的有效抑制剂

Hepatitis is a medical condition characterized by inflammation of the liver. It is commonly caused by the hepatitis viruses A, B, C, D, and E. Hepatitis A virus (HAV) is highly contagious and can spread from infected individuals, through contaminated food, blood, or can also be water-borne. As per the statistics of World Health Organization (WHO), HAV infects about 1.4 million individuals each year globally. In

this research work, we have focused on identifying natural product-based potential inhibitors for the two major enzymes of HAV namely 3C proteinase (3C(pro)) and RNA-directed RNA polymerase (RdRP). The enzyme 3C(pro) plays an important role in proteolytic activity that promotes viral maturation and infectivity. RNA-directed RNA polymerase facilitate viral replication and transcription. Structure-based virtual screening was carried out using NPACT database that contains a collection of 1574 curated plant-derived natural compounds that are validated by experiments. The screening procedure identified the phytochemical Mulberrofuran W, which could bind to both the targets 3C(pro) and RdRP. The phytochemical Mulberrofuran W also had better binding affinity compared to the control compounds atropine and pyridinyl ester, which are previously identified inhibitors of HAV 3C(pro) and RdRP, respectively. The Mulberrofuran W bound 3C(pro) and RdRP complexes were subjected to 200 ns molecular dynamics simulations and were found to be stable and interacting with the active site of the enzymes throughout the course of complex MD simulations. In addition to DFT, MMGBSA studies were also performed to validate the identified potential inhibitor further. The identified phytochemical Mulberrofuran W can be considered as a new potential drug candidate and could be taken up for experimental evaluation against HAV infection.

信息来源：Sureshan Muthusamy, et al.

MOLECULAR DIVERSITY, JUN 2023. DOI: 10.1007/s11030-023-10679-7

推荐评论：

虚拟筛选、动力学模拟等计算机技术在药物领域极大的促进了活性化合物、药物先导物的发现，提高了药物发现的能力和效率。

化学图：化学空间的交互式可视化探索

JUN 2023

Exploratory analysis of the chemical space is an important task in the field of cheminformatics. For example, in drug discovery research, chemists investigate sets of thousands of chemical compounds in order to identify novel yet structurally similar synthetic compounds to replace natural products. Manually exploring the chemical space inhabited by all possible molecules and chemical compounds is impractical, and therefore presents a challenge. To fill this gap, we present ChemoGraph, a novel visual

analytics technique for interactively exploring related chemicals. In ChemoGraph, we formalize a chemical space as a hypergraph and apply novel machine learning models to compute related chemical compounds. It uses a database to find related compounds from a known space and a machine learning model to generate new ones, which helps enlarge the known space. Moreover, ChemoGraph highlights interactive features that support users in viewing, comparing, and organizing computationally identified related chemicals. With a drug discovery usage scenario and initial expert feedback from a case study, we demonstrate the usefulness of ChemoGraph.

信息来源：Kale, Bharat, et al.

COMPUTER GRAPHICS FORUM,42(3): 13-24 DOI: 10.1111/cgf.14807

推荐评论：

“一图胜千言”。通过“化学图”，科学家能够快速探索各种分子，如天然化合物、药物等的化学空间，特别是未知的化学空间。

扩大生物信息学数据应用以对 MarinolideA 和 B——由一株化学上特殊的海洋细菌产生的 24-和 26-元大环内酯的全立体结构指认

Marinolides A and B, two new 24- and 26-membered bacterial macrolactones, were isolated from the marine-derived actinobacterium AJS-327 and their stereostructures initially assigned by bioinformatic data analysis. Macrolactones typically possess complex stereochemistry, the assignments of which have been one of the most difficult undertakings in natural products chemistry, and in most cases, the use of X-ray diffraction methods and total synthesis have been the major methods of assigning their absolute configurations. More recently, however, it has become apparent that the integration of bioinformatic data is growing in utility to assign absolute configurations. Genome mining and bioinformatic analysis identified the 97 kb mld biosynthetic cluster harboring seven type I polyketide synthases. A detailed bioinformatic investigation of the ketoreductase and enoylreductase domains within the multimodular polyketide synthases, coupled with NMR and X-ray diffraction data, allowed for the absolute configurations of marinolides A and B to be determined. While using bioinformatics to assign the relative and absolute configurations of natural products has

high potential, this method must be coupled with full NMR-based analysis to both confirm bioinformatic assignments as well as any additional modifications that occur during biosynthesis.

信息来源：Kim, Min Cheol, et al. MARINE DRUGS，21（6） 文献号: 367
DOI: 10.3390/md21060367 出版年: JUN 2023

推荐评论：

综合生物信息学和经典波谱解析等多种方法解决复杂大环内酯的构型确定难题。

利用分子动力学模拟结果训练神经网络模型有效预测环六肽结构集合

Cyclic peptides have emerged as a promising class oftherapeutics.However, their de novo design remains challenging,and many cyclic peptide drugs are simply natural products or theirderivatives. Most cyclic peptides, including the current cyclic peptidedrugs, adopt multiple conformations in water. The ability to characterizecyclic peptide structural ensembles would greatly aid their rationaldesign. In a previous pioneering study, our group demonstrated thatusing molecular dynamics results to train machine learning modelscan efficiently predict structural ensembles of cyclic pentapeptides.Using this method, which was termed StrEAMM (Structural Ensembles Achieved by Molecular Dynamics and Machine Learning), linear regression models were ableto predict the structural ensembles for an independent test set with R (2) = 0.94 between the predicted populations forspecific structures and the observed populations in molecular dynamicssimulations for cyclic pentapeptides. An underlying assumption inthese StrEAMM models is that cyclic peptide structural preferencesare predominantly influenced by neighboring interactions, namely,interactions between (1,2) and (1,3) residues. Here we demonstratethat for larger cyclic peptides such as cyclic hexapeptides, linearregression models including only (1,2) and (1,3) interactions failto produce satisfactory predictions (R (2) = 0.47); further inclusion of (1,4) interactions leads to moderateimprovements (R (2) = 0.75). We show thatwhen using convolutional neural networks and graph neural networksto incorporate complex nonlinear interaction patterns, we can achieve R (2) = 0.97 and R (2) =0.91 for cyclic pentapeptides and hexapeptides, respectively.

信息来源： Hui, Tiffani, et al.

JOURNAL OF CHEMICAL THEORY AND COMPUTATION, DOI: 10.1021/acs.jctc.3c00154

推荐评论：

机器学习模型在化合物结构方面具有非常好的应用前景。

天然产物发现的先进方法：生物活性筛选、去重复、代谢组学分析、基因组测序、数据库和信息工具以及结构阐明

2023-05-19

Natural Products (NP) are essential for the discovery of novel drugs and products for numerous biotechnological applications. The NP discovery process is expensive and time-consuming, having as major hurdles dereplication (early identification of known compounds) and structure elucidation, particularly the determination of the absolute configuration of metabolites with stereogenic centers. This review comprehensively focuses on recent technological and instrumental advances, highlighting the development of methods that alleviate these obstacles, paving the way for accelerating NP discovery towards biotechnological applications. Herein, we emphasize the most innovative high-throughput tools and methods for advancing bioactivity screening, NP chemical analysis, dereplication, metabolite profiling, metabolomics, genome sequencing and/or genomics approaches, databases, bioinformatics, chemoinformatics, and three-dimensional NP structure elucidation..

信息来源：Susana P Gaudêncio，et al.

Mar Drugs, 2023, 21(5):308. doi: 10.3390/md21050308.

https://pubmed.ncbi.nlm.nih.gov/37233502/

推荐评论：

利用多种方法解决去重复并导向发现高活性天然产物是高效发现先导物的重要途经。天然产物研究方法的快速发展对于推动天然产物科学具有深远的影响。

人尿酸转运蛋白 1（hURAT1）抑制剂的虚拟筛选和活性评价

Hyperuricemia is a disease caused by disorder of purine metabolism, mainly due to insufficient renal excretion of uric acid. Urate transporter 1 (URAT1) is the most widely studied target of urate transporters, and used for uric acid (UA) reabsorption. This study used the AlphaFold2 algorithm to predict the structure of URAT1. Virtual screening and biological evaluation were used to discover novel URAT1 inhibitors that target the critical amino acids. Seven compounds were screened from the T2220 database and validated as URAT1 inhibitors by cell biology experiments. The IC50 values of benbromarone, NP023335, TN1148, and TN1008 were 6.878, 18.46, 24.64, and 53.04 μM, respectively. Molecular dynamics simulation was used to investigate the binding mechanism of URAT1 to NP023335, which forms stable contact with Ser35, Phe365, and Arg477. These interactions are essential for maintaining the biological activity of NP023335. The three compounds' pharmacokinetic characteristics were predicted, and NP023335's properties matched those of an empirical medication with the benefits of high solubility, low cardiotoxicity, good membrane permeability, and oral absorption. The natural product NP023335 will serve as a promising hit compound for facilitating the further design of novel URAT1 inhibitors.

信息来源：Yacong Yang, et al. RSC Advances, 2023,(6), in press. https://pubs.rsc.org/en/content/articlelanding/2023/ra/d2ra07193b#!

推荐评论：

运用人工智能技术可加速基于蛋白结构的活性分子预测和先导物发现。

人工智能：天然产物药发现的虚拟化学家

2023-05-26

Nature is full of a bundle of medicinal substances and its product perceived as a prerogative structure to collaborate with protein drug targets. The natural product’s (NPs) structure heterogeneity and eccentric characteristics inspired scientists to work on natural product-inspired medicine. To gear NP drug-finding artificial intelligence (AI) to confront and excavate unexplored opportunities. Natural product-inspired drug discoveries based on AI to act as an innovative tool for molecular design and lead discovery. Various models of machine learning produce quickly synthesizable mimetics of the natural

products templates. The invention of novel natural products mimetics by computer-assisted technology provides a feasible strategy to get the natural product with defined bio-activities. AI's hit rate makes its high importance by improving trail patterns such as dose selection, trail life span, efficacy parameters, and biomarkers. Along these lines, AI methods can be a successful tool in a targeted way to formulate advanced medicinal applications for natural products. 'Prediction of future of natural product based drug discovery is not magic, actually its artificial intelligence'

信息来源：Shefali Arora,et al. Journal of Biomolecular Structure and Dynamics

推荐评论：

*运用人工智能技术将加速天然产物在新药先导物发现中的应用。

*天然产物研究的科研范式正在经历重要变革，而人工智能将在这场变革中扮演重要角色。

近期会议与活动

时间	题目	地点	相关链接
2023 年 8 月 26 日-28 日	亚太区域中医药天然产物资源创新国际研讨会	天津	http://www.tib.cas.cn/tzxx/tzgg/202307/t20230714_6810529.html
2023 年 10 月 15 日-20 日	The XXIII International Conference on Organic Synthesis	上海	https://www.163.com/dy/article/IAE0CN0G0511CTRH.html
2023 年 11 月 10-12 日	第十六届海洋药物学术年会	杭州	https://acmp2023.sciconf.cn/cn/web/index/
July 30 - August 4, 2023	Natural Products: Inspiring Innovation in Chemistry, Biology and the Discovery of New Medicines	Andover, NH, United States	https://www.grc.org/natural-products-and-bioactive-compounds-conference/2023/
25-26 Oct 2023	33rd International Conference on Nutraceuticals and Natural Medicine	Zurich, Switzerland	https://www.clocate.com/international-conference-on-nutraceuticals-and-natural-medicine/86508/
14-16 September 2023	2nd International Conference on Natural products, Medicinal Plants, and Traditional Medicines	Berlin, Germany	https://www.clocate.com/international-conference-on-natural-products-medicinal-plants-and-traditional-medicines/99760/

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人工智能与天然药物动态监测快报

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