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SUN'IY INTELLEKT VA BIOMOLEKULAR MODELLASHTIRISH- DORI ISHLAB CHIQARISHDA AI MING IMKONIYATLARI

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Annotatsiya. Ushbu maqolada sun'iy intellekt (AI) va dori vositalarini ishlab chiqishda biomolekulyar modellashtirish imkoniyatlari muhokama qilinadi. Dori-darmonlarni ishlab chiqish jarayoni ko'pincha uzoq va qimmatga tushadi; ammo AI texnologiyalarining integratsiyasi bu jarayonni tezlashtirish va samaradorligini oshirish uchun katta imkoniyatlarni taqdim etadi. Biomolekulyar modellashtirish biologik molekulalarning tuzilishi va xatti-harakatlarini taqlid qilish uchun hisoblash usullaridan foydalanadi. AI algoritmlari, xususan, mashinani o'rganish texnikasi katta ma'lumotlar to'plamini tahlil qilishda yordam beradi va yangi dori birikmalarining biologik maqsadlar bilan qanday o'zaro ta'siri haqida aniq prognozlar berishi mumkin. Maqola turli misollar orqali oqimni modellashtirish, tuzilmani bashorat qilish, virtual skrining va dori birikmalarini optimallashtirishda AIning rolini ta'kidlaydi. Bundan tashqari, u dori vositalarini ishlab chiqish jarayonida AIning muammolari va kelajakdagi istiqbollarini muhokama qiladi.

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Искусственный интеллект и биомолекулярное моделирование – потенциал ИИ в разработке лекарственных препаратов.

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Аннотация. В данной статье рассматривается потенциал искусственного интеллекта (ИИ) и биомолекулярного моделирования в разработке лекарственных препаратов. Процесс разработки лекарственных препаратов зачастую длительный и дорогостоящий; однако интеграция технологий ИИ открывает значительные возможности для ускорения этого процесса и повышения его эффективности. Биомолекулярное моделирование использует вычислительные методы для моделирования структуры и поведения биологических молекул. Алгоритмы ИИ, в частности, методы машинного обучения, помогают анализировать большие наборы данных и могут обеспечивать точные прогнозы взаимодействия новых лекарственных соединений с биологическими мишенями. В статье на различных примерах рассматривается роль ИИ в моделировании потоков, прогнозировании структуры, виртуальном скрининге и оптимизации лекарственных соединений. Кроме того, обсуждаются проблемы и перспективы применения ИИ в процессе разработки лекарственных препаратов.

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Artificial intelligence and biomolecular modeling – the potential of AI in drug development.

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Annotation.This article discusses the potential of artificial intelligence (AI) and biomolecular modeling in drug development. The drug development process is often lengthy and expensive; however, the integration of AI technologies offers significant opportunities to accelerate this process and enhance its efficiency. Biomolecular modeling utilizes computational methods to simulate the structure and behavior of biological molecules. AI algorithms, particularly machine learning techniques, assist in analyzing large datasets and can provide accurate predictions about how new drug compounds interact with biological targets. The article highlights the role of AI in

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flow modeling, structure prediction, virtual screening, and drug compound optimization through various examples. Additionally, it discusses the challenges and future prospects of AI in the drug development process.

Key words:DSP-1181,CureMetrix,DeepMind and AlphaFold,BenevolentAI.

The Transformative Role of Artificial Intelligence and Biomolecular Modeling in Drug Development.The quest for new and effective drugs is a cornerstone of modern medicine, yet the journey from initial discovery to market-ready treatment is notoriously lengthy and expensive. Traditional drug development can take over a decade and cost billions of dollars, with a high rate of failure along the way. However, the integration of artificial intelligence (AI) and biomolecular modeling is poised to revolutionize this process, offering innovative solutions that can significantly accelerate drug discovery and enhance its efficiency. Understanding Biomolecular Modeling.Biomolecular modeling employs computational techniques to simulate the structures and behaviors of biological molecules, such as proteins and nucleic acids. By creating detailed models of these biomolecules, researchers can gain insights into their functions and interactions with potential drug compounds. This modeling is crucial in understanding how drugs will behave in a biological system before they are synthesized and tested in the lab. The Power of AI in Drug Development.AI technologies, particularly machine learning algorithms, are transforming the landscape of drug development. These algorithms can analyze vast datasets generated from various sources, including genomic data, clinical trials, and previous research findings. By identifying patterns and making predictions about how new drug compounds will interact with biological targets, AI significantly reduces the time and resources required for drug discovery.

1. Flow Modeling: AI can optimize the flow of information and processes within drug development pipelines. By predicting which compounds are most likely to succeed based on historical data, researchers can prioritize their efforts and allocate resources more effectively.
2. Structure Prediction: One of the most promising applications of AI is in predicting the three-dimensional structures of proteins and other biomolecules. Tools like AlphaFold have demonstrated remarkable accuracy in predicting protein structures, which can guide the design of new drugs that target specific proteins involved in diseases.
3. Virtual Screening: AI-driven virtual screening allows researchers to evaluate thousands of potential drug candidates quickly. Instead of synthesizing and testing each compound in the lab, AI can predict which compounds are most likely to bind effectively to a target protein, significantly speeding up the initial stages of drug discovery.
4. Drug Compound Optimization: Once promising candidates are identified, AI can assist in optimizing their chemical structures to improve efficacy, reduce side effects, and enhance bioavailability. Machine learning models can analyze the relationship between molecular structure and biological activity, enabling researchers to refine their compounds systematically.Despite the immense potential of AI and biomolecular modeling in drug development, several challenges remain. Data quality and availability can vary significantly across different studies, which may affect the reliability of AI predictions. Additionally, integrating AI into existing workflows requires substantial investment in technology and training for researchers. Ethical considerations surrounding data usage and algorithmic bias also need to be addressed to ensure equitable access to these advancements. Future Prospects.As AI technologies continue to evolve, their integration into drug development processes is expected to deepen. Ongoing advancements in machine learning techniques, coupled with improved computational power, will likely lead to even more accurate predictions and faster drug discovery timelines. Collaborations between pharmaceutical companies, academic institutions, and tech firms will be critical in harnessing these innovations effectively. The Transformative Role of Artificial Intelligence and Biomolecular Modeling in

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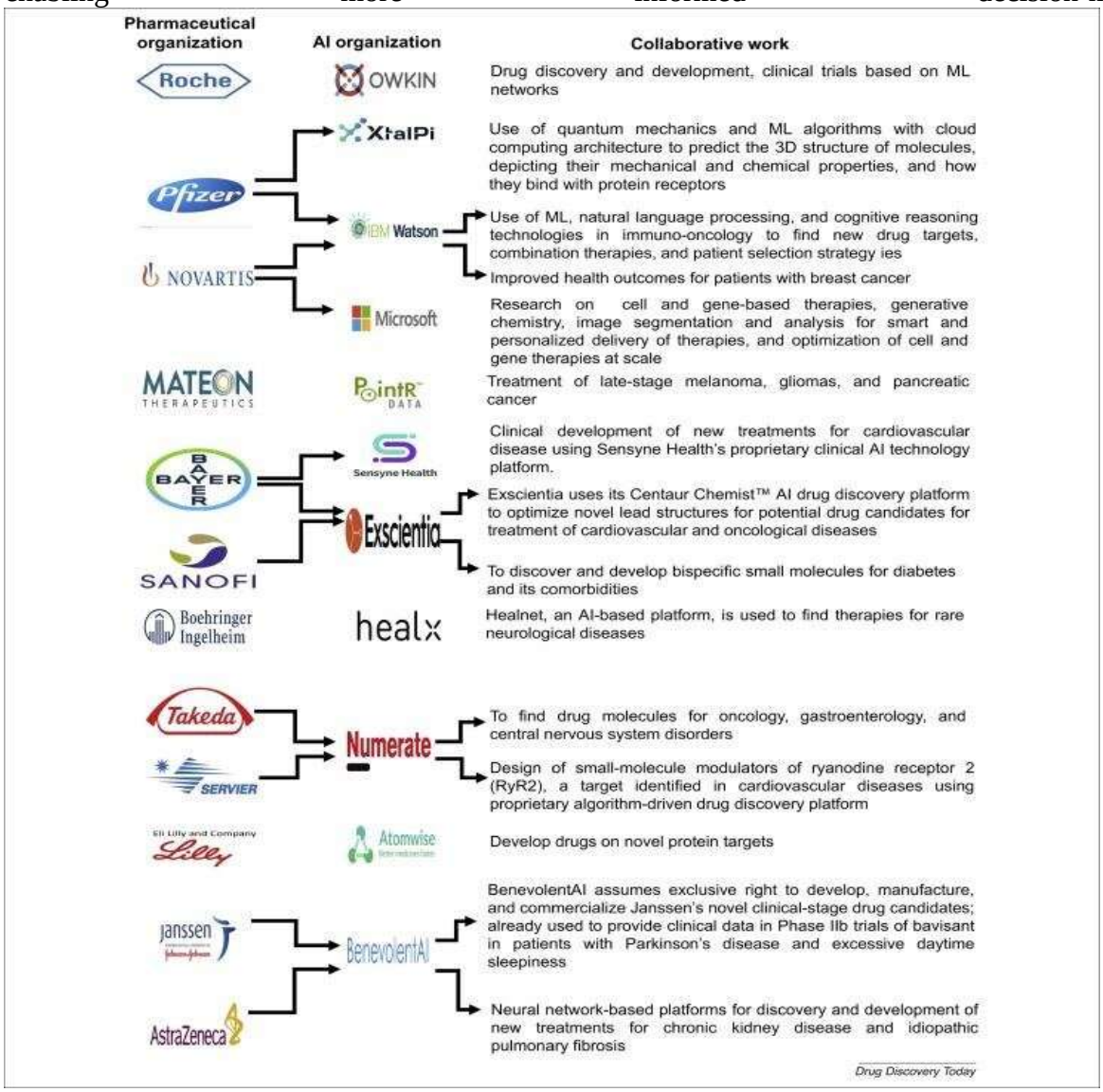
Drug Development.The landscape of drug development has been fundamentally transformed by advancements in technology, particularly through the integration of artificial intelligence (AI) and biomolecular modeling. These innovations have not only accelerated the drug discovery process but also enhanced the precision and efficacy of therapeutic interventions. This article explores how AI and biomolecular modeling are reshaping the pharmaceutical industry, driving efficiency, reducing costs, and improving outcomes. The Challenges of Traditional Drug Development.Traditionally, drug development is a lengthy and expensive process, often taking over a decade and costing billions of dollars. High attrition rates during clinical trials, primarily due to safety concerns or lack of efficacy, pose significant challenges. The need for innovative approaches to streamline this process has become increasingly urgent. The Role of Artificial Intelligence. 1. Data Analysis and Prediction: AI algorithms can analyze vast datasets from genomics, proteomics, and clinical trials to identify potential drug candidates and predict their success. Machine learning models can uncover patterns that human researchers might overlook, enabling more informed decision-making.



2. Compound Screening: AI accelerates virtual screening by predicting the binding affinity of compounds to target proteins, significantly reducing the time and resources spent on laboratory experiments. Techniques such as deep learning have shown promise in identifying novel

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compounds with desired biological activity.AI facilitates the development of personalized medicine by analyzing patient data to tailor treatments based on individual genetic profiles. This approach enhances the likelihood of treatment success and minimizes adverse effects. AI can optimize clinical trial design by identifying suitable patient populations, predicting outcomes, and even monitoring patient adherence. This leads to more efficient trials and faster time-to-market for new therapies.Artificial Intelligence (AI) is revolutionizing traditional drug discovery and development models by seamlessly integrating data, computational power, and algorithms. This synergy enhances the efficiency, accuracy, and success rates of drug research, shortens development timelines, and reduces costs. Coupled with machine learning (ML) and deep learning (DL), AI has demonstrated significant advancements across various domains, including drug characterization, target discovery and validation, small molecule drug design, and the acceleration of clinical trials. Through molecular generation techniques, AI facilitates the creation of novel drug molecules, predicting their properties and activities, while virtual screening optimizes drug candidates. **DSP-1181** is a drug developed by Insilico Medicine and created with the help of artificial intelligence. It is primarily intended for the treatment of depression and other mental disorders. This drug has undergone clinical trials, and its efficacy is being studied.**CureMetrix**: This company creates models that help in the development of new drugs in the field of oncology using artificial intelligence. They utilize AI technologies to detect and treat diseases such as breast cancer. A2A receptor antagonists: Atomwise has successfully identified new compounds as A2A receptor antagonists using artificial intelligence. These compounds are being considered as potential drugs for Parkinson's disease and other neurological disorders.**DeepMind and AlphaFold:** DeepMind's AlphaFold program has achieved revolutionary breakthroughs in predicting protein structures. This is of significant importance in identifying target proteins for drug development and in the development of new drug compounds. **BenevolentAI**: This company has achieved several successes in creating new drug compounds using artificial intelligence. They utilize AI to discover and develop new therapeutic agents for various diseases."

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