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Role of Artificial Intelligence in Simulation and Therapeutics in Neurodegenerative Diseases

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Abstract

Neurodegenerative diseases, such as Alzheimer's disease, Parkinson's disease, Huntington's disease, etc., are a cause of significant mortality rates due to a lack of curative treatments and their complex nature. Traditional therapeutic methodologies have several disadvantages such as slow diagnosis and a lack of effective treatments. They mainly focused on the management of the disease rather than curing it. The integration of artificial intelligence in the simulation and therapeutics of neurodegenerative diseases has offered a revolutionary explication. Artificial intelligence models provide early diagnosis, accurate disease modeling, and optimized drug development. Machine learning and deep learning are subsets of artificial intelligence that examine massive datasets from biomarkers, genomics, and neuroimaging to recognize trends in disease progression and suggest personalized treatments. Diagnosis precision can be elevated by agent-based modeling, predictive modeling, and image analysis. In therapeutics, artificial intelligence aids in drug repurposing, de novo drug development, personalized medicine, and the development of nanomedicine to overcome the challenge of crossing the blood–brain barrier. Artificial intelligence facilitates the development of personalized medicine by altering the treatments according to the patient's genomic clinical data, enhancing the effectiveness and minimizing the aftereffects. Irrespective of these advancements, challenges, like data quality, model understandability, and regulatory barriers, still exist. To enable the widespread application of artificial intelligence, these challenges should be addressed. Due to its ability to perform real-time diagnosis, biomarker supervision, and clinical trials, Artificial Intelligence has an optimistic future in the simulation and therapeutics of neurodegenerative diseases. Artificial intelligence can transform the healthcare industry by delivering more accurate, accessible, and reliable therapies that will optimize patient outcomes and quality of life. This article reviews various artificial intelligence tools that are used in the therapeutics and simulation of neurodegenerative disorders.

Keywords: Artificial intelligence, biomarkers, blood–brain barrier, clinical trials, deep learning, imaging, machine learning, nanomedicine, neurodegenerative diseases, personalized medicine

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INTRODUCTION

Associations of neurological diseases that cause fatalities among millions of people worldwide and imply a reduction of neurons from the central nervous system (CNS) and peripheral nervous system (PNS) are termed neurodegenerative disorders (NDD). Consequences of the disintegration of the composition and activity of CNS and PNS include malfunctions in cognitive behavior, communication systems, sensory, and motor functions, and memory loss [1].

Some examples of NDDs are Alzheimer's disease (AD), which is characterized by the production of amyloid-beta plaques and tangles of tau proteins; symptoms include loss of memory, behavioral changes, and cognitive decline [2]. Another disease is Parkinson's disease (PD), in which the dopaminergic neurons of the substantia nigra region of the brain are damaged; its symptoms include tremors, rigidity, and postural instability [3]. Huntington's disease (HD) is also an example of NDD in which repeated expansion of CAG protein in the HTT gene is observed; symptoms include cognitive decline, psychiatric issues, and motor dysfunction [4].

For the treatment of NDDs, traditional methods include pharmacological treatments (such as cholinesterase inhibitors, NMDA receptor antagonists, and dopaminergic medications), physical therapies, behavioral therapies, surgical, and device-based treatments, and immunomodulatory drugs [5]. The focus of traditional methods was on controlling the symptoms rather than the rehabilitation of the NDD. They had menacing side effects, fleeting effects, were expensive, and had access obstacles. These drawbacks accentuate the importance of introducing modern technology such as AI drug discovery or nanomedicine [6].

Artificial intelligence (AI) refers to the rapidly evolving field of computer science capable of performing tasks that would typically be solved by human intellect. AI has several implementations in healthcare systems, diagnosis, decision-making, medical imaging, drug discovery and development, and surgical and predictive practices. AI can consume, evaluate, and publish results for large amounts of data in various ways to aid in disease diagnosis and inform clinical conclusions [7].

Studies have shown that employing the integration of AI and machine learning (ML) techniques yields powerful results. For instance, AI-powered image analysis techniques have demonstrated strong results in aiding the early detection of AD. Deep learning (DL) techniques, inspired by the structure and function of the human brain, predominate in natural language processing (NLP) and image recognition, making them suitable for examining large medical data [8].

This review is a comprehensive study of the applications of AI in the simulation of NDD and its therapeutic applications. Along with AI, the use of ML and DL is making its way in the healthcare sector, as explained. The challenges and ethical issues related to the use of AI in NDD simulation and therapeutics are also discussed. Finally, there is a discussion regarding the future of AI in the healthcare business.

AI IN HEALTHCARE

AI is revolutionizing the healthcare industry by introducing ML and DL-driven technologies for diagnosis and imaging, disease simulation, drug development, personalized medicine, robotic surgery, and providing chatbots for virtual assistance, etc.

AI in medical imaging enhances the precision, effectiveness, and convenience of the disease simulation process. DL-integrated AI techniques are used to examine medical images produced by magnetic resonance imaging (MRI) scans and X-rays. These algorithms can locate peculiarities, like tumors, and they often outperform human radiologists in diagnosis. These techniques provide immediate analysis, facilitating faster identification and treatment of diseases. It also assists in recognizing urgent cases, thereby streamlining the prioritization process for treatment [9].

AI modifies personalized treatment by delivering therapies specifically designed for individual patients based on their genetic makeup and clinical and lifestyle data. It explores various data, including medical history, genomics, and biomarkers of the patient, and prescribes refined drug dosage and targeted therapies. AI-driven personalized medicines reduce the risk of side effects and pave the way for more effective treatment. Integrating AI with wearable devices makes healthcare more dynamic and patient-oriented [10].

AI is contributing to drug development by encouraging discovery, making it budget-friendly, and enhancing efficacy. ML models assist in detecting drug targets, anticipating compound potency, and creating fresh molecules. AI narrows down preclinical studies by predicting toxicity and detecting biomarkers. AI validates drug reformulation by uncovering new uses for existing drugs. AI is introducing reviving therapies by making drug development faster and more productive [11].

Introducing AI in surgery, as robotic surgery is revolutionizing, as it improves accuracy, productivity, and results. AI provides immediate analysis and feedback, detects sensitive structures, and enhances incision points. AI contributes to developing three-dimensional models from imaging datasets for pre-surgical strategy. AI minimizes complexities and healing periods. Amid obstacles, such as expenses and regulatory hurdles, AI is revolutionizing robotic surgery by minimizing internal procedures, enhancing protection, and laying the foundation for completely independent surgeries in the future [12].

Hence, AI is transforming healthcare by integrating ML and DL into various sectors. AI improves speed, accuracy, and quicker diagnosis, and designs customized treatments according to patients' requirements. AI economizes and repurposes pre-existing drugs. AI is making healthcare more systemic and patient-oriented and laying the foundation for an independent and individualized medical system.

AI-DRIVEN DISEASE MODELING AND SIMULATION

Early diagnosis of NDD and anticipatory management are crucial to alleviating unfavorable outcomes. It allows the identification of disease biomarkers and risk factors before the disease symptoms surface, allowing early and personalized treatment [13]. AI incorporates multiple data sources, like biosensors, cognitive evaluations, and neuroimaging, to enhance NDD simulation. Using ML, NLP, and predictive analysis, AI identifies patterns, simulates disease progression, and provides personalized treatment.

Fiber Bragg Grating (FBG) is a biosensor widely recognized in the medical field for its high susceptibility, moldability, and multi-channel functionality. FBGs can be employed to observe heart rate, temperature, and body movement, indicative signs of NDD, especially PD, with AI analytics. ML interprets the data, parallel to imaging and genetic profiles, to simulate disease progression [14].

Diffusion kurtosis imaging (DKI), a diffusion MRI technique that produces metrics, like mean kurtosis, indicates microstructural complexity and can detect slight changes in tissue that are not detectable through orthodox diffusion matrices. DKI has recognized changes in grey matter in regions, like the hippocampus in PD and AD, and its susceptibility ranges to white matter pathways crucial for sensory and integrative processing [15].

Machine Learning for Biomarker Analysis

Recent investigations focus on the role of biomarkers, such as exosomes and miRNA in the presymptomatic stage of NDD, to detect neuronal malfunction. However, conventional methods for detecting these biomarkers can be expensive and presumptuous and can only be performed at specific centers [16]. These drawbacks make the integration of modern technology necessary for biomarker detection. Electroencephalography (EEG) is an application of ML that has proven exceptional in the prognosis of NDD. Many researchers have highlighted some unique methods for EEG-based diagnosis that include hybrid deep neural networks, partial directed coherence, and wavelet entropy analysis. Lately, studies have implemented the use of the fractal dimension as a feature descriptor of an ML workflow for the diagnosis of PD [17].

Another technique, diffusion tensor imaging (DTI) with MRI, imparts details about the microstructural transmutations of the white matter of the CNS. DTI detects early white matter deterioration in AD by inspecting water diffusion patterns in brain tissues [18].

ML amplifies AD diagnosis by analyzing cerebrospinal fluid (CSF) biomarkers, such as neurofilament light chain, phosphorylated tau, total tau, and amyloid-β with the help of models, such as random forest. Incorporating CSF with MRI will enhance precision. The integration of CSF with ML is computerized, flexible, and insightful. It differentiates AD from other dementias [19].

Deep Learning for Image Analysis

DL is a subset of AI that implies multifaceted artificial neural networks to operate on data. DL can perform tasks like image recognition, decision-making, and prediction generation [20].

For the classification of NDD, we can utilize QR-represented gait data. Gait data, when converted into QR codes and categorized using a convolutional neural network (CNN), will distinguish between PD and HD. This procedure simulates that encrypting gait data as QR will give a two-dimensional representation that can accentuate CNN's capability to identify and categorize disease-specific gait patterns [21].

Functional magnetic resonance imaging (FMRI) is a non-surgical approach to diagnosing NDD. FMRI data can detect aberrations or malfunctions in large-scale brain function networks via altered functional connectivity analysis [22].

Agent-Based Modeling and Artificial Intelligence

In an agent-based model, neurons act in a liberated, independent, and self-driven manner. This model has proved to have an important application in healthcare as it involves community outreach.

A new multi-agent-based model called the multiple feature evaluation approach (MFEA) has been put forward by recent studies. It analyzes multiple data sources, like genomics, biomarkers, neuroimaging, and patient history, to improve simulation precision and risk anticipation. MFEA, by integrating the aforesaid attributes with sophisticated algorithms and ML models, detects complicated disease trends and relations. This technique allows for quicker diagnosis, customized treatment planning, and better patient results. This multifaceted analysis is pivotal for comprehending disease pathways and NDD exploration [23].

Another technique, statistical reduction approach with deep hyper-optimization (SRADHO), is a modern AI model for disease categorization. It incorporates statistical feature reduction to terminate disturbance and improve applicable data, enhancing model competence. By adjusting neural network variables, deep hyper-optimization optimizes performance and minimizes overfitting. By combining these approaches, SRADHO boosts forecasting performance, accelerates development, and allows accurate disease systemization, which is more productive for NDD diagnosis [24].

Predictive Modeling of Neurodegenerative Disease Progression

The development of predictive models based on advanced neural networks has proved to be extremely preferable for both the early detection of NDD and precise diagnosis. These models provide rapid and accurate diagnosis by employing neural networks' adaptability and capability to detect complicated trends in patient data. Using predictive analysis gives customized recommendations for therapeutic interventions, which leads to better medication plans for better patient results.

The PREDICT-HD model is created for the early diagnosis and supervision of HD. It combines neuroimaging, analytical, clinical trials, and biomarker data to anticipate disease emergence. By examining longitudinal data, the model detects negligible changes before symptoms surface. It authorizes sophisticated ML algorithms and improves diagnostic precision by allowing customized interventions. This model assists in comprehending disease pathways and provides support for therapeutic development for HD [25].

The integration of long short-term memory networks (LSTM), random forest, and gradient boosting machines (GBM) provides an influential perspective on NDD diagnosis and development prediction.

LSTM dominates in recognizing temporal trends in longitudinal datasets such as biomarker change and cognitive impairment. Random forest improves endurance and accessibility by handling high-dimensional data and optimizing feature selection. GBM optimizes prediction accuracy, enhancing model performance. This integration of all three models imposes the power of all three algorithms to provide a thorough, precise, and reliable tool for early diagnosis and personalized therapies for NDD treatment [26].

Artificial Intelligence-Powered Image Analysis for Animal Models

AI-powered image analysis for animal models of NDD employs sophisticated algorithms to optimize disease comprehension and therapeutic development. DL approaches accurately identify and evaluate changes like neurofibrillary tangles, neuronal loss, and amyloid plaques from neuroimaging and histological data. It permits high-quality investigations by reducing human errors and speeding up the research process.

Integrating genomics, clinical phenotyping, and neuroimaging is crucial for implementing a three-dimensional diagnostic model for NDD simulation and personalized medicine. Genomics examines any genetic defects and molecular targets, neuroimaging identifies any change in the structure and function of the brain, like tumors, and clinical phenotyping gives brief symptom assessment and progression trends. The model provides a complete, personalized disease assessment by combining the above-mentioned aspects of the AI algorithm. This approach facilitates precise diagnosis, personalized therapeutic interventions, and improved patient outcomes in NDD [27].

ARTIFICIAL INTELLIGENCE-DRIVEN THERAPEUTICS

The introduction of AI in therapeutics for NDD has proven a transforming step in accelerating drug development by analyzing large amounts of data to recognize new potential drug targets and reprocess existing drugs. ML enhances the effectiveness and defense of the drug by modifying chemical structures, whereas DL contributes to early disease markers by biomarker analysis or neuroimaging [28].

The development of personalized medicine is done by altering the treatments based on the patient’s genetic profile and trends in disease emergence. AI also came up with the development of nanoparticles that can cross the blood–brain barrier, which guarantees targeted drug delivery with the least after-effects. AI optimizes CRISPR-CAS9 accuracy, allowing targeted genetic modifications in gene therapy for diseases like HD.

These advancements depict the revolutionary capability of AI for the treatment of NDDs, laying the foundation for more accessible, customized, and reliable therapies.

Target Identification and Validation

For target identification and validation of drug development, AI algorithms incorporate and examine data from various sets like genomics and metabolomics. ML models identify trends and relations that are difficult to detect manually, uncovering potential therapies. AI also maps protein and gene interactions to comprehend disease mechanisms of NDD like in AD. AI detects key proteins involved in disease emergence. DL models examine biomarker fluids and neuro-imaging data to detect preliminary evidence of the disease; validation of these biomarkers helps to confirm the applicability of drug targets [29].

AI-powered models, like neural networks, anticipate the consequences of drug targets. ML models estimate the reciprocity between potential drugs and targets, enhancing their binding affinity and reducing harmful effects. This boosts the effectiveness of drug development in NDD.

Netra AI is an emerging AI model for drug target identification and validation that analyzes elaborate biological data sets. It tracks gene and protein communication networks to reveal disease pathways and possible drug targets. It also authenticates biomarkers associated with early NDD development. Its AI-powered simulation estimates the impact of drugs, reduces costs for trials, and speeds up the drug development process for more productive and customized treatment for NDD [30].

The integration of molecular docking with DL models optimizes drug target identification and validation. AI models examine biological data to recognize prospective therapeutic targets, whereas molecular docking estimates the binding affinity of the possible compound. This method speeds up the drug development process by anticipating drug-target reciprocity with more precision. Hybrid neural network for drug target affinity is an example of a hybrid neural network model that integrates various encoding networks to enhance binding affinity estimation and paves the way for the selection of the most favorable drug. This synchronization between AI and molecular docking is making way for novel therapies for NDD [31].

Drug Repurposing

The transformation of drug repurposing in drug development by AI for NDD therapeutics is expanding the recognition of prevailing drugs with prospective novel uses. Using ML models, AI explores multiple biological data to detect disease mechanisms and therapeutic targets linked with NDDs like AD, PD, etc. AI models devise the drug-target reciprocity and anticipate the effectiveness of sanctioned drugs on these targets, reducing duration and expenses compared to conventional drug development methodologies.

To unwrap the concealed association between the drug and disease pathways, DL models, like neural networks and NLP, go through scientific literature, medical experiment data, and health records. For instance, memantine, and metformin have been recognized for prospective repurposing of AD and PD, respectively, by AI. Moreover, AI also imitates drug-disease reciprocity to estimate the therapeutic results, enhancing drug mixtures for increased effectiveness and minimizing after-effects. This technique accelerates and increases the effectiveness of drug development. By authorizing AI-driven drug repurposing, scientists can develop fast, safe, reliable, and budget-friendly drugs for NDD treatment [32].

An AI framework, interpretable few-shot predictive task meta-learning (IFPTML), is an optimistic ML model for drug repurposing in the treatment of NDD. Contrary to conventional DL models, this model is brilliant in handling small datasets. By using pre-existing data and recognizing new drug candidates with small data, IFPTML adjusts according to numerous NDDs. Its explicability optimizes the comprehension ability of the mechanism of action, helping in the research of the biomarker-drug relationship using multi-omics data. Moreover, IFPTML enhances drug-target interaction anticipation by examining binding affinity, lethality, and similarity to drugs [33].

De Novo Drug Design

A transforming invention of innovative treatments for NDDs, like AD, PD, etc., is AI-driven de novo drug design, which yields completely novel molecules upgraded for target selectivity, blood–brain barrier permeability, and reduced lethality. Reinforcement learning regulates molecular structure to enhance similarity with drugs, whereas novel compounds with enhanced therapeutic properties can be developed by AI-powered models like generative adversarial networks (GANs). Prediction of drug-target reciprocity can be improved by structure-based drug design using tools like molecular docking. AI also combines multi-omics data to reveal new targets for drugs, allowing a customized technique for NDD therapies [34].

AI can develop non-lethal dual-specificity tyrosine-regulated kinase 1A inhibitors for the treatment of AD using GAN models by enhancing properties like reducing lethality, bioavailability, and blood–brain barrier permeability. The quantitative structure-activity relationship (QSAR) model anticipates the binding affinity, whereas directed message passing neural networks perform potential toxicity evaluation. New inhibitors are promoted by the hierarchical graph generation model and clarified using molecular docking [35].

Regardless of obstacles, like a lack of data and clinical authentication, the integration of AI with wet lab can speed up the development of novel drugs for NDD therapeutics.

Personalized Medicine

To develop a personalized treatment for the patients of NDDs, like AD, PD, etc., AI first classifies them into subgroups based on their genomic, biological, and clinical data. For this purpose, ML and DL models go through large multi-omics data to anticipate disease emergence. For instance, CNN can analyze MRI or CT scan data to recognize any structural changes in the brain and can distinguish between subtypes of AD [36].

For an effective treatment, it is important to monitor the patient's response to the drugs given. In NDDs, every patient responds differently to treatments due to diversity in factors like metabolism, disease emergence, and genetic makeup. AI models increase the precision of medicine by altering treatments according to every patient's description. Pharmacogenic AI models scrutinize genetic variability affecting drug effectiveness, enabling doctors to alter treatment. Reinforcement learning models can facilitate drug formulation for greater satisfaction [37].

AI helps in enhancing vectors for gene therapy, which is important for NDD therapeutics. AI improves CRISPR-based treatments by anticipating off-target effects and safer gene editing for diseases like HD. Generative AI models create viral vectors for gene delivery, enhance target selectivity, and minimize the immune response menace [38].

AI also improves the effectiveness of clinical trials, enhancing the accuracy of prediction and trial design. To find out about the eligible participants for the trial, NLP extracts clinical data from health records. For versatile and maximum outcomes, AI models allow adaptive clinical trials. ML algorithms inspect the biomarker data to enhance treatment effectiveness and identify early signals for safety.

Artificial Intelligence in the Development of Nanomedicine

AI is accelerating the design, enhancement, and delivery of nanoparticle-based drugs for NDD treatment. AI models aid in developing biocompatible nanoparticles, improving blood–brain barrier penetration, and predicting drug loading effectiveness. By anticipating solubility, stability, and drug-loading capacity, AI enhances the development of nanoparticles. ML algorithms examine extensive datasets to recognize the suitable nanocarrier characteristics such as size, shape, surface charge, and functionalization for effective brain targeting. DL models optimize nanoparticle design by estimating how nanocarriers communicate with disease-specific targets [33].

AI models, like graph neural networks and reinforcement learning, predict amendments in nanoparticles to improve blood–brain barrier permeability to overcome the obstacle of crossing the blood–brain barrier. AI-driven models strengthen nanoparticles, like exosomes, dendrimers, and PEGylated liposomes, to ensure the effortless transmission of nano drugs into the central nervous system. Furthermore, the fabrication of nanoparticles that particularly bind to misfolded proteins to ensure precise drug delivery is made feasible by AI-driven molecular docking simulations [39].

AI models enhance lethality estimation and biological compatibility evaluation with the help of DL and QSAR models that examine massive data to anticipate safety, immune responses, and long-term effects of nanoparticles. This authorizes the scientists to exclude prospective lethal nanoparticles in the initial developmental stages to minimize the hazardous effects in clinical trials [40].

Integrating AI with nanomedicine has encouraged the development of more productive, customized, and safer treatments for NDD. The evolution of AI models will play a momentous role in facilitating the development of nanodrugs, target-specific delivery, and enhancing clinical results for patients of NDD.

CHALLENGES ASSOCIATED WITH THE USE OF ARTIFICIAL INTELLIGENCE

The application of AI in NDD simulation and therapeutics has made several important advancements in the diagnosis, patient stratification, drug discovery, and development of personalized medicine for the simulation and therapeutics of NDD. However, several obstacles are preventing the widespread adoption and efficacy of AI in the healthcare industry [41].

The accessibility and quality of the data are a major challenge. The AI model needs massive, high-quality data, but the data available for NDD is inadequate, uneven, and insufficient. Patient variations may affect neuroimaging, clinical, and genomic data, conflicting diagnostic benchmarks, and discrepancies in data compilation across different study groups [42].

Another challenge is the ability of AI to comprehend data. Many DL models act as “black boxes”, making it difficult for researchers to implement AI-driven recommendations. Explainable AI is required to ensure that AI-driven estimations and suggestions are explicit, comprehensible, and clinically applicable [43]. AI also faces challenges with the external validation of the data. Scarcity of external validation and consistency restricts the clinical reiteration of AI algorithms, making them unreliable for real-world applications [44].

In drug discovery and development, the AI-generated prospective drug requires massive external validation, which is expensive and time-consuming. In the lab, AI-predicted drugs display a high affinity for NDD targets; however, in vivo, in vitro, and clinical trials show the ineffective action of these drugs [45]. Another challenge can be associated with the approval of regulatory bodies, as AI-powered drug discovery does not hold standardized approval frameworks from agencies like the FDA [46]. Lastly, many institutions lack the infrastructure to implement AI-powered diagnosis, biomarker examination, and treatment improvement, hence making it challenging to combine AI with clinical workflows. Health workers are required to be trained to translate AI outputs, and AI algorithms should be easily integrated with electronic health record systems [47].

To conquer these challenges, structured datasets, external validation, explainable AI, improved clinical integration, and regulatory approval are required. Overcoming these challenges will assist in achieving its full potential in transforming NDD diagnosis and therapeutics.

FUTURE ASPECTS AND CONCLUSION

AI in the application of simulation and therapeutics of NDDs represents a revolutionary upturn due to its ability to provide early and real-time diagnosis, precise biomarker analysis, the ability to comprehend data quickly, and in the development of personalized medicine. With the assistance of AI algorithms, like disease progression modeling and neural network simulations, we can now easily simulate the behavior of neural networks to figure out the extent of cellular and molecular levels of NDD. DL models can integrate with imaging techniques, like MRI and CT scans, to detect the NDD at early stages. For biomarker analysis, wearable devices can be developed with AI algorithms that can monitor changes in biomarkers associated with NDD such as tau proteins and amyloid beta. For drug development, AI can integrate with omics techniques to recognize new drug targets. AI can also help in drug repurposing by analyzing the potential effectiveness of existing drugs for NDDs, reducing the time and cost of drug development. AI can also go through patients’ data to alter the treatment suitable for each patient. AI models can also help with the identification of preferred candidates for drug testing, enhancing protocols for trial design. AI models can also analyze real-world data to boost clinical trial results and pave the way for long-term efficiency of the treatment.

Nevertheless, challenges, like data quality, regulatory obstacles, and model understandability, are there. The need for external validation and the “black box” nature of AI restricts their widespread application. The involvement of explainable AI and its implementation with clinical workflow have successfully addressed such issues.

AI holds the capability to revolutionize NDD healthcare by providing accessible, accurate, and constructive treatments as it develops, enhancing the quality of life for patients worldwide.

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