REVIEW ARTICLE

AI AND MACHINE LEARNING IN BIOTECH: DRUG DISCOVERY, EPIGENETICS & DISEASE PROGNOSIS

Meenakshi Johri*, Bindu Rajaguru, Apurva Singh and Sumeet Sannak

Pillai College of Arts, Commerce and Science (Autonomous),

New Panvel, Navi Mumbai

Corresponding author E-mail: m.johri101@gmail.com

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Abstract:

Artificial Intelligence (AI) and Machine Learning (ML) are quickly changing the way we approach biotechnology. In this review, we look at how these technologies are being used in three major areas: drug discovery, epigenetics, and disease prognosis. In drug development, AI helps scientists find potential drug targets, design new drug molecules, and predict how well a drug might work all in less time and at lower cost than traditional methods.

In the field of epigenetics, which studies changes in gene activity without changing the DNA sequence, AI tools help researchers understand complex data. These tools can find patterns in things like DNA methylation and histone modifications, which are important for understanding how genes are turned on or off in different diseases.

AI is also becoming more common in predicting and diagnosing diseases. By analysing data from medical records, genetic tests, and even medical images, AI can help doctors detect diseases early, predict how serious they might become, and choose the best treatments for each patient. This is especially useful in conditions like cancer, heart disease, and neurological disorders.

This article brings together recent developments and examples to show how AI and ML are being used in these areas. It also talks about some of the challenges, like making sure the data is accurate, the models are easy to understand, and the technology is used responsibly. As AI continues to improve, it has the potential to make biotechnology and healthcare faster, smarter, and more personalized.

Keyword: Artificial Intelligence, Machine Learning, Epigenetics, Prognosis, Drug Discovery, Personalized Medicine.

Introduction:

Biotechnology is one of the most exciting and fast-growing areas of science today. It plays a major role in improving healthcare, developing new medicines, and helping us understand how our bodies work at the genetic level. But as the science becomes more advanced, researchers are faced with an overwhelming amount of complex data. Traditional methods though still important are often too slow or limited to handle this information effectively. This is where Artificial Intelligence (AI) and Machine Learning (ML) are beginning to make a real difference.

AI and ML are computer-based technologies that can "learn" from data and help make predictions or decisions. Instead of telling the computer exactly what to do, we give it data and let it figure out patterns and solutions on its own. These tools are already being used in many industries, but their impact on biotechnology has been especially powerful in recent years.

One area that has changed significantly because of AI is drug discovery. Creating a new drug used to take 10–15 years and cost a huge amount of money. Now, with the help of AI, researchers can quickly scan through massive libraries of molecules, predict which ones might work, and test them using simulations all before entering a real laboratory. This saves time, money, and opens doors to finding treatments for diseases that were previously too complex to tackle.

Another important field is epigenetics, which looks at how genes are turned on or off not by changing the DNA itself, but by chemical signals that control gene activity. AI helps scientists explore these tiny changes in our cells, understand their role in diseases like cancer, and even discover new biomarkers that could lead to earlier diagnosis or better treatments.

AI is also helping doctors and scientists improve how we predict and diagnose diseases. By analysing things like genetic data, medical images, and patient records, AI can often spot warning signs earlier than humans can. These tools are already being used in hospitals to help identify risks, personalize treatment plans, and improve patient outcomes, especially in conditions like cancer, heart disease, and neurological disorders.

1. The Role of AI And Machine Learning in Drug Discovery

The process of discovering new drugs has always been a time-consuming, expensive, and uncertain journey. Traditionally, scientists had to rely heavily on trial-and-error experiments, slow lab procedures, and years of clinical research to bring a single drug to the market. It's a pathway filled with high costs, long timelines, and many failures. However, the landscape of drug discovery has started to shift in a dramatic way, thanks to the growing involvement of artificial intelligence (AI) and machine learning (Deng *et al*., 2021).

In the simplest terms, AI refers to computer systems that can mimic human intelligence things like learning from experience, recognizing patterns, and making decisions. Machine learning is a branch of AI that focuses on teaching computers to learn from data, identify trends, and improve over time without needing explicit instructions for every step. In the world of drug discovery, these technologies have become powerful tools for researchers, helping to solve problems that were once too big, too complex, or too slow to tackle using traditional approaches (Alizadehsani *et al*., 2023).

a. A New Approach to an Old Problem

The traditional drug discovery pipeline is long and difficult. It starts with identifying a biological target, such as a protein or gene that plays a role in a disease. From there, researchers design or find compounds that might interact with this target. These compounds go through laboratory testing, then animal trials, and eventually, human clinical trials. For every drug that succeeds, there are thousands that fail somewhere along the way. The entire process can take over 10 years and cost more than a billion dollars (Deng *et al.*, 2021).

AI and ML are offering ways to speed up this process, cut costs, and improve success rates. These technologies are especially good at dealing with large amounts of complex data something that modern biology and chemistry produce in abundance. From analyzing genomic data to screening chemical libraries, AI helps researchers focus their efforts on the most promising candidates much earlier in the process.(Raschka & Kaufman, 2020)

b. Target Identification and Validation

One of the first steps in drug discovery is figuring out what to target in the body. This might be a malfunctioning protein in cancer, a viral enzyme in an infection, or a genetic mutation in a rare disease. But with thousands of possible targets in the human body, how do scientists decide where to start?

This is where AI truly shines. By analysing huge datasets, like those from genomic studies, protein databases, and patient records. AI systems can identify patterns that suggest which targets are most likely to play a role in a particular disease. For example, machine learning algorithms can detect relationships between gene mutations and disease symptoms, helping researchers prioritize the most relevant biological pathways (Qiu & Wei, 2023) that used to take months of literature review and lab work can now be done in a fraction of the time, thanks to AI's ability to process massive amounts of information quickly and accurately.

c. Drug Design and Molecular Screening

Once a target is identified, the next step is to find or design a compound that can bind to it and modify its activity in a helpful way. This is often compared to finding the right key to fit a specific lock. Traditionally, researchers would test thousands of compounds to see which ones worked an expensive and time-intensive process.

Today, AI can dramatically narrow the search. Using deep learning models and neural networks, scientists can virtually “screen” millions of molecules in silico (on a computer) to predict how well they might bind to a target. This virtual screening process helps filter out weak or harmful candidates before they ever reach the lab. Beyond that, AI can also design entirely new molecules from scratch. By learning the rules of chemistry and structure-activity relationships from existing data, AI tools can suggest novel molecular structures that are likely to be both effective and safe. This opens the door to creating drugs that have never existed before tailor-made to treat specific diseases (Alizadehsani *et al.*, 2023).

d. Repurposing Existing Drugs

AI is also helping in drug repurposing- that is, finding new uses for old drugs. Because these drugs have already been approved for use, they can often be brought to market more quickly and

cheaply than brand-new ones (Raschka & Kaufman, 2020).

By scanning through databases of approved drugs, disease profiles, and biological pathways, AI systems can spot unexpected connections. For example, a drug originally developed for high blood pressure might also show promise in treating migraines or even certain cancers. This approach has gained attention during global health emergencies, like the COVID-19 pandemic, where speed was critical (Guo *et al*., 2024).

e. Optimizing Clinical Trials

Clinical trials are the final and most expensive stage of drug development. They involve testing the drug on real patients to measure safety and effectiveness. But organizing these trials is complicated. Choosing the right participants, designing the study, and analysing results all take time and careful planning.

AI is making this easier too. Algorithms can help identify the best candidates for a trial based on genetic data, past health records, and other factors. This ensures that the results are more accurate and that fewer people need to be exposed to experimental treatments unnecessarily. AI tools can also track how patients are responding during the trial, spotting issues early and even suggesting changes to the protocol in real-time. This kind of adaptive trial design has the potential to make studies faster, cheaper, and more ethical (Alizadehsani *et al*., 2023).

f. Real-World Examples

Several pharmaceutical companies and research labs are already using AI in their drug development pipelines. For instance, companies like Insilico Medicine, Benevolent AI, and Atomwise are developing AI platforms to discover new drug candidates at record speeds. Some of the drugs discovered with the help of AI are already in clinical trials, and a few have even reached the market (Deng *et al*., 2021).

During the COVID-19 crisis, AI played a crucial role in identifying potential treatments, analysing the virus's genetic structure, and helping researchers around the world share findings quickly.

2. The Role of AI and Machine Learning in Epigenetics

Epigenetics is the study of how genes are turned on or off without changing the actual DNA sequence. These changes called "epigenetic modifications" can happen due to aging, lifestyle, diet, pollution, or disease. Even though the DNA stays the same, these small chemical changes can affect how cells behave, how diseases develop, and how treatments work. That's what makes epigenetics such an exciting and fast-growing area in biotechnology (Guo *et al*., 2024).

However, studying epigenetics is not easy. The information involved is incredibly complex. Each human cell contains around 3 billion DNA base pairs, and the patterns of gene regulation differ between tissues, stages of development, and disease conditions. Traditional lab techniques can only take us so far when dealing with this many data. This is where Artificial Intelligence (AI) and Machine Learning (ML) are becoming powerful tools for researchers. These technologies can process massive datasets, spot patterns that human eyes might miss, and even make predictions based on very subtle changes in the data. Let's look at how AI and ML are helping scientists better understand epigenetics and how this is leading to big improvements in diagnostics, treatments, and even personalized medicine

(Guo *et al*., 2024).

a. Analysing Complex Epigenetic Data

In epigenetics, scientists study things like DNA methylation, histone modifications, and chromatin accessibility. These chemical tags control how tightly DNA is packed, and which genes are active or silent. Collecting this information involves technologies like ChIP-seq, ATAC-seq, and DNA methylation arrays. These experiments generate huge amounts of raw data, which can be overwhelming. AI helps by: Sorting through this data quickly, identifying significant patterns in gene regulation and Finding areas of the genome that might be important in certain diseases (Alizadehsani *et al*., 2023).

b. Discovering Epigenetic Biomarkers

An epigenetic biomarker is a chemical change in DNA or chromatin that can be used to detect disease, predict how severe it will become, or monitor how well treatment is working. AI models are trained using data from healthy and diseased individuals. Once trained, these models can: Detect small but meaningful changes in epigenetic marks, differentiate between disease subtypes, Help identify who is at risk for certain conditions, even before symptoms appear.

This is especially useful for early-stage cancers, where DNA methylation patterns can give away the presence of tumours long before they are large enough to be detected by scans. In diseases like Alzheimer's, diabetes, or autoimmune disorders, where early detection is difficult, AI-powered epigenetic analysis could become a game-changer (Raschka & Kaufman, 2020).

c. Linking Epigenetics to Environmental and Lifestyle Factors

One of the most fascinating parts of epigenetics is that it shows how our environment and lifestyle affect our genes. Factors like smoking, diet, exercise, pollution, and stress don't change our DNA, but they can leave marks on our genome through epigenetic modifications.

For example, AI can help find out how long-term exposure to air pollution affects gene expression in lung cells, or how childhood stress influences brain development through epigenetic changes (Zamnova, 2019).

d. Supporting Personalized Epigenetic Medicine

Every individual's epigenetic makeup is unique. Two people with the same disease may have different gene expression patterns and may respond differently to the same treatment. AI and ML are now being used to build personalized epigenetic profiles that help:

- Tailor treatments to individual patients.
- Predict how a person will respond to a drug.
- Reduce trial-and-error in prescribing medications.(Gopalan *et al*., 2023)

Let's say a cancer patient has a tumour with a certain methylation signature. An AI model can compare this profile with data from other patients and suggest the treatment that worked best for similar cases. This is a huge step toward precision medicine, where treatments are based not just on the disease, but on the biology of each person.

3. The Role of AI and Machine Learning in Disease Prognosis

In the world of medicine, being able to predict how a disease might behave in the future is a

big advantage. Doctors have always tried to do this based on their knowledge, patient symptoms, and test results. But now, with the growing use of Artificial Intelligence (AI) and Machine Learning (ML), we have smarter and faster ways to understand what might happen next in a patient's health journey (Deng *et al*., 2021).

AI and ML are technologies that can study large amounts of health data like blood tests, X-rays, MRIs, patient records, and even genetics and learn patterns from them. These patterns help in making predictions about how a disease may progress. For example, they can identify if a cancer might grow quickly, if a heart condition could lead to a heart attack, or if diabetes might cause complications in the future. These predictions are not based on guesswork they are backed by studying thousands or even millions of similar cases from the past.

a. Early Detection of Diseases

AI and machine learning are excellent at spotting health issues before symptoms even appear. These technologies can look at medical records, blood reports, scans, and even genetic data to find small signs that something might be going wrong in the body. This allows doctors to catch diseases like cancer, diabetes, or heart problems in the very early stages when they're much easier to treat. Early detection can save lives and reduce the cost and stress of treatment (Zamnova, 2019).

b. Predicting Disease Progression

Once a person is diagnosed with a disease, the next big question is: *what's going to happen next?* Will it get worse quickly, stay stable, or improve? AI can help answer that. By learning from past patient data, it can predict how fast a disease might progress in someone and what complications could come up. This is very useful in long-term conditions like Parkinson's, kidney disease, or multiple sclerosis, where the course of illness varies from person to person.

c. Personalized Prognosis for Every Patient

One of the most impressive aspects of AI is its ability to offer personalized predictions. It doesn't treat everyone the same. Instead, it studies each person's age, gender, health history, genetics, habits, and other personal factors to give tailored insights. For example, two patients with the same cancer may have very different treatment responses and AI can help doctors understand who might respond better and why. This level of personalization leads to better and more effective care (Alizadehsani *et al*., 2023).

d. Real-Time Monitoring and Alerts

Wearable devices like smartwatches, fitness trackers, and health monitors are now being paired with AI to keep an eye on people's health in real time. These tools track things like heart rate, oxygen levels, sleep patterns, or blood sugar and AI looks at this data continuously. If something unusual is detected, it can send alerts to both the patient and the doctor, allowing immediate action. This is especially helpful for elderly patients, those with heart issues, or people with chronic conditions (Deng *et al*., 2021).

e. Predicting Treatment Outcomes

AI also helps predict how well a certain treatment might work for a particular patient. It analyses data from similar cases to estimate the success rate of surgeries, medicines, or therapies. This

helps doctors make more informed decisions, avoid treatments that might not work, and try options that have a higher chance of success. For example, in cancer therapy, AI can guide whether a patient will respond better to chemotherapy, radiation, or a combination of both (Raschka & Kaufman, 2020).

f. Reducing Human Error and Bias

Doctors, like all humans, can sometimes make mistakes or carry unconscious biases. AI can help reduce these risks by relying strictly on data. It doesn't get tired, emotional, or distracted.

If trained properly, it can provide consistent, objective evaluations. This is especially useful in busy hospitals or during emergencies when decisions need to be made quickly and correctly.

Applications of AI and Machine Learning in Drug Discover, Epigenetics and Disease Prognosis:

Artificial Intelligence (AI) and Machine Learning (ML) have become powerful tools in the world of biotechnology. Their ability to quickly analyse massive datasets, recognize patterns, and make predictions is changing how scientists and doctors approach diseases from finding new drugs to understanding gene expression, and even predicting how a disease will behave in a patient (Raschka & Kaufman, 2020).

Applications in Drug Discovery:

AI and ML are helping discover and develop new medicines faster, cheaper, and more accurately than traditional methods.

- Target Identification: AI algorithms analyse biological data to find which genes or proteins are involved in a disease. This helps researchers choose the right targets to develop drugs against (Kumar *et al.*, 2023).
- Drug Candidate Screening: Machine learning models can screen thousands of chemical compounds and predict which ones are most likely to bind to the target and be effective. This saves time and avoids expensive lab testing.
- Predicting Drug Behaviour: AI tools can forecast how a drug will behave in the body how it gets absorbed, metabolized, and whether it might be toxic. This helps avoid failure in later trial stages (Deng *et al.*, 2021).
- Drug Repurposing: Instead of starting from scratch, AI looks for existing drugs that could be used for new diseases (for example, using a cancer drug for COVID-19). This approach is faster and less risky (Raschka & Kaufman, 2020).
- Clinical Trial Optimization: AI helps design smarter clinical trials by identifying suitable patient groups, predicting side effects, and monitoring trial data in real time.

Applications in Epigenetics:

AI and ML are unlocking the secrets of epigenetic changes those chemical modifications that control gene activity without changing the DNA sequence.

- Understanding DNA Methylation and Histone Modifications: AI tools can analyse huge epigenetic datasets and spot patterns in DNA methylation or histone changes that are linked to diseases, especially cancers (Raschka & Kaufman, 2020).
- Identifying Epigenetic Biomarkers: ML models help detect unique epigenetic signals that can be used to diagnose diseases early or monitor treatment effectiveness.

- Single-Cell Epigenomics: Modern technologies like single-cell RNA-seq generate massive data. AI is essential for organizing and interpreting this data to understand how individual cells behave differently in health and disease (Sanghvi *et al.,* 2024).
- Linking Epigenetics to Gene Expression: AI connects the dots between epigenetic changes and how genes turn on or off, which is key to understanding complex diseases like autoimmune disorders, neurological diseases, and cancer.

Application in Disease Prognosis:

AI and ML are making it possible to predict how diseases will develop in patients, enabling more proactive and personalized care.

- Early Disease Prediction: By analysing health records, genetic information, lifestyle data, and even wearable device readings, AI can predict who is at risk of developing diseases like diabetes, heart disease, or Alzheimer's.(Qiu & Wei, 2023)
- Forecasting Disease Progression: ML models can monitor how a disease evolves over time. For example, AI can predict if cancer will spread, if diabetes will lead to kidney failure, or how fast Parkinson's disease will worsen.
- Personalized Treatment Plans: AI tailor predictions to each person's unique profile, helping doctors choose the most suitable treatments, adjust doses, and monitor for side effects.(Alizadehsani *et al.*, 2023)
- Real-Time Monitoring: With the help of smart devices and AI algorithms, patients can be continuously monitored. If something abnormal is detected, alerts can be sent to doctors or caregivers.

Challenges and Limitations:

While AI and Machine Learning have brought impressive progress in biotechnology, they are not without limitations. These technologies are powerful, but they still face challenges that need to be addressed especially when used in sensitive areas like drug development, gene research, and patient care.

1. **In Drug Discovery**
    - Data Quality and Availability: Drug discovery depends on large volumes of chemical, biological, and clinical data. But often, this data is scattered, incomplete, or not standardized. If the data used to train AI models is poor, the predictions will be unreliable.(Kumar *et al*., 2023)
    - Lack of Experimental Validation: AI can suggest new drug candidates or predict how they might work but these predictions still need lab testing and clinical trials. Without experimental follow-up, AI discoveries remain just theoretical.
    - Black-Box Problem: Many AI models (especially deep learning) work in a way that is hard to interpret. They may give a result but not clearly explain how they arrived at it. In drug discovery, this can be risky because researchers need to understand the science behind a decision.(Deng *et al.*, 2021)
    - High Cost of Implementation: Developing and integrating AI into the drug discovery

pipeline often requires costly infrastructure, high-performance computing, and skilled personnel something not all research labs or companies can afford.

2. **In Epigenetics**
   - Complexity of Epigenetic Data: Epigenetic information is highly dynamic and varies across different cell types, tissues, and even between individuals. Training AI to make sense of this complexity is extremely difficult.(Sanghvi *et al.*, 2024)
   - Limited Public Datasets: Unlike genetic data, which has many open databases, high-quality epigenetic data is still limited. This restricts the ability of AI models to generalize well across different conditions and populations.(Qiu & Wei, 2023)
   - Interpreting Results: Even if AI detects epigenetic patterns, understanding what they mean biologically isn't easy. Many connections between epigenetic marks and diseases are still being studied, making validation a challenge.
   - Single-Cell Analysis Bottlenecks: AI is used for single-cell sequencing, but the volume and complexity of this data can overwhelm current models. Training algorithms to work accurately on noisy, sparse data from single cells remains a technical hurdle.*(Deng et al.,* 2021)
3. **In Disease Prognosis**
   - Data Privacy and Security: Patient data used in prognosis models is highly sensitive. Using this data requires strict regulations to protect patient privacy, and not all institutions have the safeguards or policies in place.(Qiu & Wei, 2023)
   - Bias in AI Models: If the training data is biased such as being mostly from one ethnic group, gender, or region the AI model might give skewed results. This can lead to inaccurate predictions, especially for underrepresented populations.(Kumar *et al.,* 2023)
   - Over-Reliance on AI: There is a growing concern that too much trust may be placed in AI predictions, especially in critical situations. Doctors must balance AI insights with human judgment, but sometimes, AI can influence decisions more than it should.
   - Lack of Explainability: Patients and healthcare providers may hesitate to accept AI- driven prognosis tools if the system cannot clearly explain why a particular outcome or risk was predicted. Transparency is essential for trust.(Raschka & Kaufman, 2020)

Future Prospects:

The journey of artificial intelligence (AI) and machine learning (ML) in biotechnology is just getting started. While current applications have already made impressive contributions, the true potential of these technologies lies in what's ahead. The future promises not only faster scientific breakthroughs but also a transformation in how we approach health, disease, and treatment at a deeply personal level. As tools become more advanced and data more accessible, AI and ML are expected to bring revolutionary changes in drug development, epigenetic understanding, and disease prediction (Qiu & Wei, 2023).

Future of AI & ML in Drug Discovery

In the coming years, AI is expected to streamline drug development even further, minimizing

the time and cost required to bring a new medicine to market.

- AI-Designed Molecules: AI will move beyond screening existing compounds and start creating completely new chemical structures based on specific disease targets.
- Smarter Clinical Trials: AI will help design and adapt clinical trials in real-time, identifying the best patient groups and modifying protocols as new data is gathered.
- Predicting Human Response: ML models will become better at predicting how drugs interact with human biology, improving the chances of success and reducing harmful side effects.
- Quantum + AI in Drug Design: The integration of quantum computing may allow for precise simulation of molecular behaviour, making drug discovery even faster and more accurate.
- Global Drug Accessibility: AI can be used to repurpose affordable, existing drugs for rare or neglected diseases offering solutions where traditional pharma doesn't reach (Sanghvi *et al.*, 2024).

Future of AI & ML in Epigenetics

Epigenetics is all about understanding how genes are switched on and off and AI is poised to unlock this complex code in ways human researchers can't do alone.

- Personalized Epigenetic Profiles: AI will help build individual maps of epigenetic markers, revealing personal risk factors and guiding custom treatment plans.
- Early Detection of Disease: Changes in gene expression often occur before symptoms show. AI models may be able to detect disease at its earliest stage, even before standard tests can.
- AI-Guided Epigenetic Editing: As gene-editing tools become more precise, AI could identify the safest and most effective spots for epigenetic interventions offering potential cures without altering the DNA itself (Kumar *et al.,* 2023).
- Deeper Understanding of Complex Illnesses: Diseases like cancer, diabetes, and Alzheimer's are influenced by both genes and environment. AI will help us understand how epigenetic changes contribute to these diseases in a more detailed and predictive way (Alizadehsani *et al.*, 2023).

Future of AI & ML in Disease Prognosis

In the future, disease prognosis will become less about treating illness after it appears, and more about preventing it from developing in the first place.

- Real-Time Health Monitoring: With the help of AI, wearable devices and mobile health apps will continuously track vitals and behaviours, predicting health problems before symptoms arise.
- AI in Predicting Mental and Neurological Disorders: AI systems may soon be able to forecast mental health relapses, seizure risks, or cognitive decline by analysing subtle changes in speech, movement, or sleep patterns.
- Home-Based Prognostic Tools: AI-powered home devices could offer disease predictions and health checkups remotely, reducing the need for frequent hospital visits.

Early Warning Dashboards: Hospitals may rely on AI dashboards that monitor patients continuously, predicting critical events hours or days in advance, and enabling timely interventions (Jadhav *et al*., 2024).

Conclusion:

Artificial Intelligence and Machine Learning are no longer just experimental tools they've become essential drivers of progress in biotechnology. In drug discovery, they are helping scientists identify targets, design molecules, and fast-track clinical trials with greater precision than ever before. In epigenetics, these technologies are unlocking complex gene regulation patterns that influence health and disease, offering new possibilities for personalized treatments. And when it comes to disease prognosis, AI and ML are making it possible to predict health outcomes early, tailor therapies to individuals, and even prevent diseases before symptoms arise.

However, while the potential is enormous, these systems are not without their challenges. Issues like data quality, algorithm transparency, and ethical concerns must be addressed to ensure safe and fair use of AI in healthcare and life sciences.

Looking ahead, the future holds exciting possibilities smarter drug pipelines, deeper genetic understanding, and truly personalized medicine. With continued innovation, collaboration, and responsible development, AI and ML are set to reshape the landscape of biotechnology, bringing us closer to a future where healthcare is faster, more accurate, and uniquely tailored to each person.

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