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Role of Artificial Intelligence in Niosomes Development

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ABSTRACT

The development of niosomes alongside other drug delivery Nano systems takes place through artificial intelligence (AI) applications that show increasing utility. The delivery of therapeutic drugs to specific locations becomes efficient through the use of niosomal methods. Drugs in niosomes exist as multi-lamellar vesicles (MLVs) and large unilamellar vesicles (LUVs) and small unilamellar vesicles (SUVs) based on their size dimensions. By examining the intricate connections between niosome characteristics and performance, AI algorithms can optimise niosome design. AI can direct the formulation process to achieve regulated drug release and increased encapsulation efficiency by forecasting and simulating drug-nano carrier interactions. By anticipating release patterns and minimising the number of optimisations runs required, artificial intelligence (AI) simplifies the drug formulation process and hence lowers labour and manufacturing costs. AI can also predict drug release, disintegration timings, and dissolution profiles, which makes it easier to choose the best batch for further scaling. Additionally, machine learning algorithms can detect dangerous structural features or forecast negative consequences. Finding illness targets for medication administration is improved by combining multi-omics data with AI-driven network analysis.

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- **Introduction:**

Current modeling of human cognitive functions through artificial intelligence (AI) has advanced dramatically in fields like drug discovery and delivery processes according to three examples [1, 2, 3]. AI adoption rates for drug development acceleration have raised the acknowledgment of efficient drug discovery hence researchers focus on this field. Drug delivery applications of AI have recently gained extensive interest because newly developed algorithms and technologies enhance drug transportation performance.

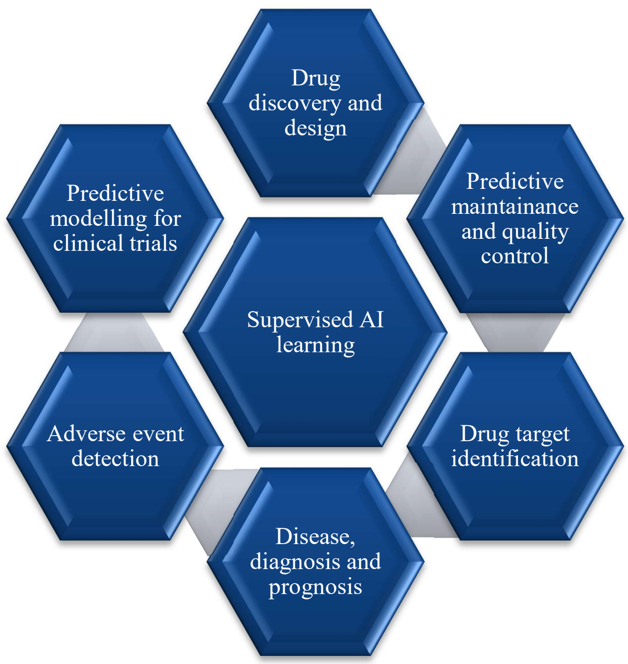
- **AI in Drug Delivery System:**

Several AI methods allow drug delivery system enhancement including drug body response prediction and formulation optimization and drug interaction prediction. Machine learning programs evaluate extensive databases documenting pharmaceutical behavior in the body which enables them to predict drug reactions. AI-based algorithms perform drug formulation enhancements which represent a prominent example in drug delivery systems. The training of these algorithms becomes easier when employing body-based medication data from large datasets to identify optimal formulations for specific medications. Using large datasets with medication interactions during neural network training allows practitioners to forecast drug-to-drug interactions. The training of neural networks through extensive databases about medication interactions enables forecasts of drug-drug interactions. The creation of drug delivery systems benefits from this functionality during development. Hydrogels together with dendrimers and nanoparticles join liposomes and microspheres in being AI-based drug delivery methods. Artificial intelligence developed drug delivery systems through innovation in drug carriers along with prediction of drug profiles and optimal drug measurements [4,5].

Machine learning together with deep learning and natural language processing are subsets that artificial intelligence uses as its methodology. The learning type between supervised and unsupervised assignment exists alongside the essential role of chosen algorithms. Supervised learning approaches enable machines to operate through known inputs and outputs because it functions differently from unsupervised learning which manages unclassified outputs. A supervised system utilizes various input characteristics along with features to estimate target results. Feature-homogeneous groupings are what unsupervised classification aims to produce [6].

1. **Supervised AI Learning:**

A pre-labelled dataset becomes essential for supervised learning because it allows an algorithm to learn through specific output training. Through analysis of labeled data the algorithm graduates into identifying proper output values for inbound data. Task-driven approaches create particular objectives that guide the production of desired results from available input data. The training of predictive algorithms relies on tagged data through this technique for both classification work and predictive fu0nctions. Supervised learning manages two main problem domains with classification and regression as the core issues. The outcome from regression models is numeric while classification models designate results through labels. The key models used include DOM Forest together with Ensemble Learning in combination with K-Nearest Neighbour and Support Vector Machines. Multiple strategies exist for dealing with supervised learning difficulties based on the data types encountered in particular problem domains. Random forest along with ensemble learning and K-nearest neighbours and support vector machines and Naïve Bayes and linear regression and support vector regression are among the different



methods used [7].

Figure 1: Supervised AI learning

The pharmaceutical industry utilizes this technology for various applications described as follows:

- **Drug discovery and design:**

Supervised learning algorithms used in drug discovery help foretell both behavioral patterns and attributes of newly designed medications. A recognized dataset with substances alongside their activities trains the model to detect patterns between molecular characteristics and expected results. New compounds can be predicted regarding their activity level and strength and toxicity properties through this method thus supporting drug development processes and formulation steps [8].

- **Predictive maintenance and Quality control:**

A supervised learning model enables pharmaceutical manufacturers to use it for quality control and predictive maintenance functions. The predictive model deduces equipment breakdowns and quality deviations and process inaccuracies through data training using actual manufacturing data points and machinery sensor readings and quality assessment results [9].

- **Identification of drug target:**

Supervised learning uses analysis of biological data to find drug target opportunities. By processing datasets with detailed information about genetic and proteomic and transcriptomic features linked to drug reaction or disease evolution the model learns to detect patterns which it uses to identify promising targets for scientific research [10].

- **Disease diagnosis and prognosis:**

Supervised learning models discover patient illnesses by diagnosing them and predicting their medical outcomes through the application of medical data. Supervised learning models study datasets containing patient details and medical data and disease outcomes to create different disease categories or predict disease developments and treatment effectiveness [11].

- **Detection of adverse events:**

Supervised learning methods can process pharmacovigilance data to identify, sort and detect adverse events that occur while using medications. The model trains on classified adverse event reports to acquire detection patterns and recognize possible safety signals that assist in adverse event research and analysis [12].

- **Predictive Modelling for Clinical Trials:**

The supervised learning method helps forecast the outcomes of clinical trials. Previous clinical trial data provides the necessary basis for the model to predict patient responses and treatment effects while determining safety outcomes after training with datasets containing patient information and treatment procedures and experimental results. Clinical trial designs become better and patient selection improves with the use of this information [13].

Supervised learning methods find multiple applications in pharmaceutical development according to the provided examples. Supervised learning techniques together with correct feature selection along with proper data preprocessing and model assessment measurements deliver useful insights for decision support from research through development to manufacturing stages of pharmaceutical work.

2. **Unsupervised AI Learning:**

Through unsupervised learning algorithms operate without getting direct instructions from human input data. The system operates independently to perceive data patterns and relations in the collected information. The approach finds usage in initial data investigations to detect concealed patterns and groupings in datasets. This data-driven strategy functions as a "data-driven approach" to detect patterns along with structures and insights in unprocessed data. The most often performed unsupervised duties consist of clustering, dimensionality reduction, visualisation, association rule discovery and anomaly detection. The following unsupervised learning problems have different solutions based on widely used approaches which include clustering algorithms (K-medoids, hierarchical clustering, K-means, complete linkage, single linkage, BOTS) and association learning algorithms and feature selection and extraction methods (principal component analysis, Pearson correlation) [14,15].

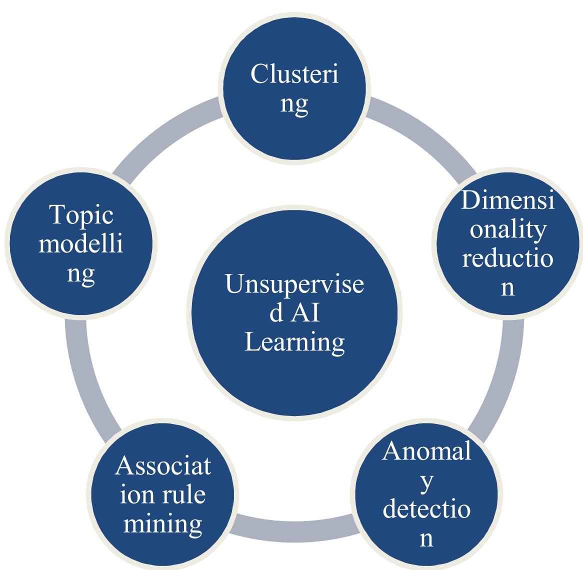


Figure 2: Unsupervised AI learning

Unsupervised learning methods in Artificial Intelligence possess three main advantages for pharmaceutical work that include exploratory analysis and pattern recognition and data visualization capabilities.

- **Clustering:**

Data detection through clustering algorithms depends on point categorization to find natural datapoint clusters which align based on similarity measures. Cluster analysis allows researchers to extract similar subgroups with shared qualities through patient data and chemical structure and gene expression profile datasets in pharmaceutical research. The identification of targets alongside patient stratification and observation of drug and illness classes forms a useful application of this method [16].

- **Dimensionality Reduction:**

The principal component analysis (PCA) and t-distributed stochastic neighbour embedding (t-SNE) tools provide solutions for reducing high-dimensional datasets while maintaining crucial information. Dimensions reduction methods assist decision support while assisting variable or feature selection and offering improved visualisation of complex data collections. The technique of dimensionality reduction delivers benefits to multiple pharmaceutical data kinds including gene expression profiles combined with drug activity profiles and medical images [17].

- **Anomaly Detection:**

The algorithms designed for anomaly detection system hunt for unique patterns that stand apart from predicted statistical models. Anomaly detection systems help pharmaceutical organizations discover errors in data quality and adverse events and possible safety hazards. Maverick detection systems located within isolation forest and the local outlier factor (LOF) enable the identification of anomalous statistics for investigation purposes [18].

- **Association Rule Mining**:

The Apropi algorithm together with other association rule mining approaches identifies important connections between included items in collections. The pharmaceutical sector applies association rule mining to assess adverse event data as well as drug-drug interactions together with patterns of concomitant drug and medical conditions. Association rule mining techniques help both pharmacovigilance studies and drug interaction discovery as well as tracking pharmaceutical market trends [19].

- **Topic Modelling**:

LDA serves as one of the topic modelling techniques used to discover hidden topics within extensive text collections. Topic modelling enables pharmaceutical industry operations to extract relevant research themes and new trends as well as patient sentiments from scientific literature and clinical trial data and social media content. The method enables pharmaceutical industry teams to conduct competitive research and collect information from literature while also learning about patient feedback [20,21].

Pharmaceutical functions benefit from unsupervised learning algorithms since they produce useful insights together with exploratory research findings. When analyzing unsupervised learning outcomes the results require domain-specific expertise and post-validation activities for obtaining meaningful data and valid conclusions

- **Role of AI in Pharmaceutical Industry:**

AI serves as an effective tool which tackles various pharmaceutical-related problems. A large body of biological data becomes usable when processed by AI algorithms that help identify disease-related targets and predict target-drug interactions [22].This allows us to approach the drug discovery process with greater focus and effectiveness. Additionally, machine learning techniques help with experiment design, pharmacokinetic and toxicity prediction, and lead compound optimisation. Consequently, there is less need for comprehensive animal experimentation. Furthermore, real-world patient data can be analysed by AI systems, enabling personalised medicine strategies. In the end, this results in better patient adherence and more successful treatment outcomes. One AI technology that improves medical treatment and lowers costs is IBM Watson, which makes it possible to diagnose and analyse data more quickly [23]. Furthermore, by making it possible to produce customised drugs, AI may improve the pharmaceutical manufacturing process. Nonetheless, issues including ethical considerations, data privacy, and regulatory guidelines must be addressed. In necessary for the pharmaceutical industry to successfully use AI.

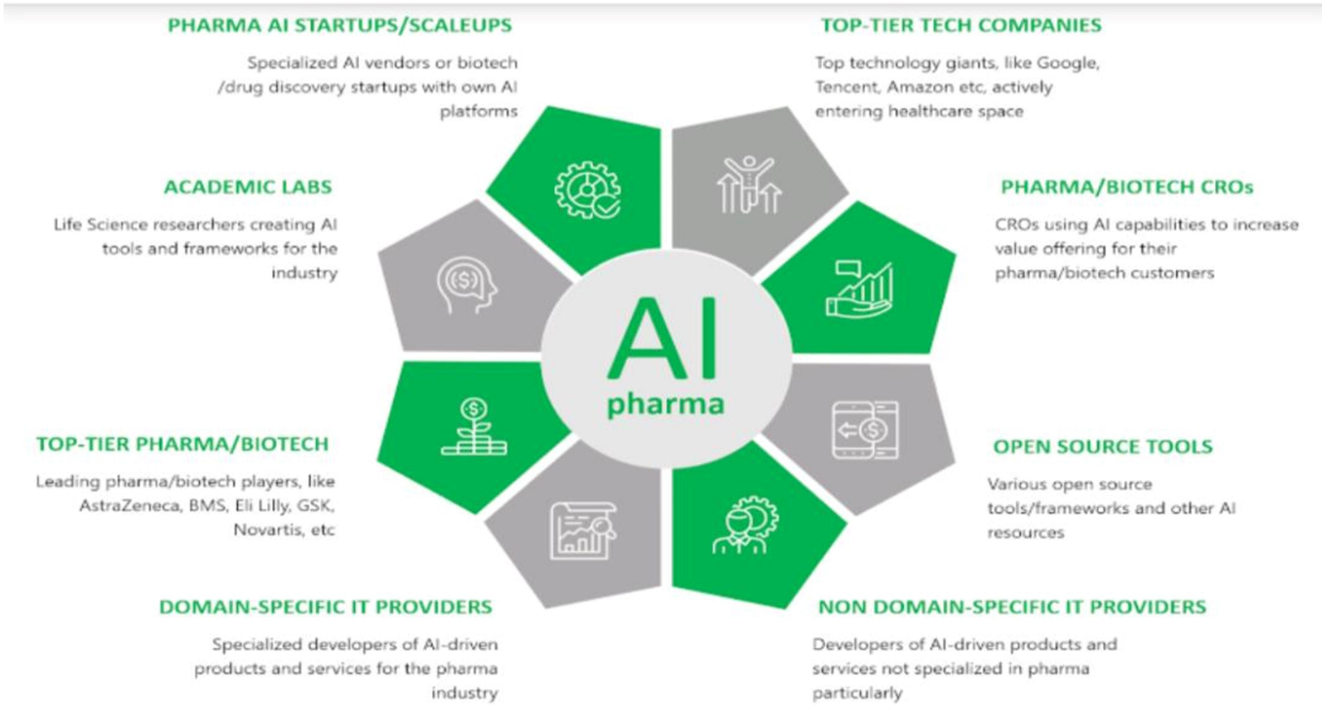


Figure 3: Role of AI in Pharmaceutical Industry

- **Prediction of Release Kinetics of Niosomal Formulation with AI:**

One area of medication delivery systems that shows promise is the use of artificial intelligence (AI) to forecast the release kinetics of niosomal formulations. Given their versatility as drug carriers, niosomes need exact control over their release characteristics in order to improve therapeutic efficacy. By using a variety of techniques to model and forecast drug release behaviours, AI can make a substantial contribution to this field.

1. Machine Learning Approaches

The capacity of machine learning methods to forecast the entrapment efficiency and release kinetics of niosomal formulations has been shown in recent research. To optimise niosomal formulations based on past data and experimental findings, for example, a machine learning framework was created to examine various parameters influencing drug entrapment and release [24,25]. These models can pinpoint intricate relationships between formulation elements that affect release kinetics, like surfactant content and drug characteristics.

2. Kinetic Modelling

To comprehend how medications are released from niosomes over time, kinetic modelling is crucial. Zero-order, first-order, Higuchi, and Korsmeyer-Peppas models are frequently employed. By identifying the best match using statistical measures like regression coefficients, AI can help fit experimental release data to these models. Some niosomal formulations, for instance, have been found to follow a Higuchi model, suggesting a diffusion-controlled release mechanism [26,27]. This fitting procedure can be automated by AI, increasing its speed and precision.

3. Simulation of Release Profiles

AI is also capable of simulating niosome release profiles under a variety of circumstances, such as temperature fluctuations and pH shifts. Researchers can forecast how the niosome structure and the drug's physicochemical characteristics will impact drug release in actual biological settings by employing computer models that take these parameters into account. Better niosomal formulation creation and optimisation for certain therapeutic uses is made possible by this capability [28, 29].

4. Data Integration and Analysis

AI methods like deep learning can improve the integration of data from several sources, including formulation factors, ambient conditions, and in vitro release experiments. This method makes it possible to create thorough predictive models that consider a greater number of factors influencing drug release kinetics [23, 30]. These models can shed light on how formulation adjustments can result in the intended release profile alterations.

- **AI-Enhanced Targeting Strategies**

The incorporation of AI into niosomal drug delivery systems can significantly improve targeting efficiency via several mechanisms:

a) **Predictive Modelling:** AI systems can analyze extensive datasets that help forecast tissue or cell interaction with niosome structures. By generating predictive power AI systems facilitate the improvement of niosome formulations to achieve better drug delivery to specific disorders.

b) **Surface Modification:** AI can help create niosomes with certain peptides or ligands that increase their affinity for target cells. For instance, research has demonstrated that adding chlorotoxin to niosome enhances their capacity to cross the blood-brain barrier and efficiently target glioblastoma cells [27,31].

c) **Real-Time Monitoring:** AI systems can help track the distribution of niosomes in the body in real time, allowing for therapeutic modifications to improve targeting effectiveness even more [32].

• Integrating Artificial Intelligence (AI) with Nanotechnology :

The pharmaceutical industry now focuses its attention on pharmaceutics and drug delivery systems because the advancement of modern molecular commodities proved to be slow and cost-intensive along with reduced productivity. The advancement of new formulations depends on costly and time-consuming conventional trials that show unpredictable results. The biomedical field developed "computational pharmaceutics" as an advanced system from modern algorithm and computing advancements during the last decade. This system merges big data with artificial intelligence (AI) and multiple scale modeling operations. The application of artificial intelligence (AI) methods becomes increasingly prevalent within pharmaceutical product development to predict release rates of drugs in test tubes along with stability characteristics and absorption details and drug-testing correlations [194]. Machine learning allowed Run Han and associates to predict the long-term physical stability of solid dispersions at three-months and six-months [33]. In 2021 Hanlu Gao and his associates conducted research on solid dispersion dissolution patterns through machine learning analysis. The predictive power of A random forest algorithm reached 85% accuracy when validated five times over different datasets using both "maintain super saturation" and "spring-and-parachute" models. This validation established equally high sensitivity and specificity levels. The Random Forest regression model achieved 7.78% mean absolute error through 5-fold cross-validation[34].

- **Predicting drug release and absorption parameters:**

The drug release and absorption parameters received accurate predictions through AI-based models. Artificial intelligence systems achieve medication release kinetic predictions by evaluating data from different drug delivery systems. AI models evaluate the drug release rate alongside pharmacokinetic scope by processing information about drug physical properties together with formulation specifics as well as delivery system release mechanics. Artificial intelligence-based models effectively predict how medications move out of numerous drug delivery systems which include oral tablets and transdermal patches and inhalers [35]. Through AI-based models healthcare professionals can anticipate the drug absorption parameters by measuring bioavailability and absorption rate according to factors such as medication solubility combined with permeability measures and formulation attributes.

The models take medicine physical characteristics along with molecular weight and lipophilicity to absorption data for assessing bloodstream penetration capability. AI-based models represent a powerful resource for predicting the forecast behavior of medicine release together with absorption characteristics. These models utilize machine learning algorithms to study diverse factors which leads to formulation optimization of medicines alongside assisting development decisions for drugs and enhancing drug delivery systems [36-42].

- **Benefits of Using AI for the Design of Niosomes**

The design and improvement of niosomes, which are vesicular drug delivery systems based on non-ionic surfactants, are increasingly using artificial intelligence (AI). There are many benefits to using AI in this field, which improves the effectiveness, safety, and efficiency of medication delivery systems.

1. Optimization of Formulation:

AI has the potential to greatly simplify the niosome formulation process. To determine the ideal compositions and circumstances for niosome manufacturing, researchers can examine enormous datasets using machine learning methods. This involves forecasting the physicochemical characteristics of various additives and surfactants, which may result in better drug release profiles and encapsulation [27,43]. The time and expense involved in developing formulations using conventional trial-and-error techniques are decreased when artificial intelligence is used.

2. Enhanced Predictive Capabilities:

Artificial intelligence (AI) algorithms can forecast the stability, release rates, and interactions of niosomes with different tissues in biological systems. To ensure that medications are released at the appropriate time and location within the body, researchers can optimize oral, topical, or injectable drug delivery pathways thanks to these predictive capabilities [27, 44]. These improvements are essential for raising therapeutic efficacy and bioavailability.

3. Improved Targeting and Efficacy:

AI can help create niosome that target tissues or cells more successfully. AI aids in the building of niosomes that may elude immune clearance and improve drug accumulation at target areas, such as tumours, by combining information on tissue properties and cellular absorption pathways [45, 46]. This focused strategy lowers systemic toxicity while also increasing efficacy.

4. Cost-Effectiveness and Scalability

Drug development procedures can be made less expensive by using AI into niosome design. Businesses can reduce production costs while preserving high standards of quality by using predictive modelling to optimize formulations and manufacturing processes [43, 44]. Furthermore, niosome production can be scaled from laboratory to industrial levels utilizing AI-driven methods without sacrificing quality.

5. Continuous Improvement Through Data Analysis

AI systems have the ability to continuously learn from fresh data produced by clinical trials or research. Better results are eventually achieved because of this continuous analysis, which enables iterative changes in niosome formulations based on actual performance data [27]. In a subject like medicine distribution that is changing quickly, this kind of flexibility is essential.

- **Recent advancements in artificial intelligence for novel drug delivery systems:**

The pharmaceutical delivery industry can transform through artificial intelligence due to its capability to enhance drug creation along with targeting and distribution aspects. New AI-controlled medication delivery systems have recently been developed in this setting.

a) **Machine learning for drug discovery:**

Nowadays, machine learning algorithms are used to analyse large datasets, find possible therapeutic targets, forecast a drug's efficacy, and improve a medicine's characteristics. With the ability to analyse millions of molecules, these AI-powered drug discovery systems can drastically cut down on the time and expense involved in medication development.

b) Nanoparticle based drug delivery systems:

Drug delivery systems based on nanoparticles: Nanoparticles can be expertly tailored to deliver medications to bodily regions or cells. AI is now being used to optimise these nanoparticles' designs to increase medication efficacy and reduce toxicity.

c) Predictive drug release models:

AI models predict drug behaviour in the body, facilitating regulated medication delivery systems. This advantageous ability ensures that medications are delivered to the body at the appropriate time and location, improving therapeutic efficacy and reducing unwanted side effects.

d) AI-powered sensors in drug delivery systems:

AI-powered sensors in drug delivery systems enable real-time monitoring, allowing doctors to customise treatment regimens and adjust medication dosages.

e) **Personalized medicine:**

By using artificial intelligence to analyse patient data, customized medicine delivery systems that consider each patient's unique physiological traits and medical history can be created. This individualized approach reduces the risk of adverse reaction and improves treatment outcomes [48].

f) Drug Repurposing:

Approved medications receive new therapeutic purposes through the method of drug repurposing which artificial intelligence performs. AI algorithms evaluate extensive data alongside biological information to detect potential therapeutic applications of existing medications for different disease treatments. The method provides an efficient and budget-friendly approach for medication development.

g) AI helps optimise drug formulation and delivery systems:

AI tools generate predictions about drug release behavior as well as substance absorption patterns which help optimize effective dosage delivery routes. AI developers use its capabilities to manufacture pharmaceutical devices which improve patient adherence together with enhanced delivery convenience.

h) **Optimal Clinical trial design :**

Clinical studies are being optimized by AI, increasing productivity and cutting expenses. AI systems can optimize trial procedures, find appropriate trial populations, and help with patient recruitment. AI also helps with real-time trial data monitoring and analysis, which enables more rapid decision-making and adaptive trial designs.

i) **Regulatory Compliance and Safety:**

AI is being utilized more and more to guarantee medication safety and assist with regulatory compliance. Artificial intelligence (AI) systems can monitor post-marketing medication safety and detect any safety concerns by analysing literature, adverse event reports, and real-world data. Additionally, AI aids in signal recognition, adverse event prediction, and pharmacovigilance.

j) Supply Chain Optimization:

Pharmaceutical supply chains are optimized using AI, which guarantees effective production, distribution, and inventory control. Artificial intelligence (AI) algorithms can improve quality control procedures, forecast demand, and optimize production schedules, all of which will lead to more efficient and economical operations.

- **Conclusion:**

The application of AI to innovative medication delivery systems has the potential to completely transform the medical industry. treatment delivery systems with AI capabilities can increase patient outcomes, decrease side effects, and increase treatment efficacy. The loss of jobs is the biggest concern about AI. Therefore, strict implementation and appropriate restrictions are required for it. However, these technologies cannot take the place of people; their sole purpose is to make life easier by facilitating smooth work. It would aid in the creation of newer medications with targeted molecules that can function on their precise place and route, reducing the likelihood of negative drug reactions and boosting their efficacy.

We can anticipate even more cutting-edge drug delivery systems that are tailored to each patient's unique requirements in terms of different novel approaches utilized to enhance the safety and effectiveness of phytomedicines and the application of novel formulations as AI technology develops. Soon, artificial intelligence will be a crucial instrument in the pharmaceutical sector. AI has a significant ability to forecast the release kinetics of niosomal compositions. Researchers can greatly improve the creation and optimization of niosomal drug delivery systems by utilizing machine learning methods for kinetic modelling, simulating release profiles under various situations, integrating diverse datasets, and enabling real-time monitoring. By guaranteeing that medications are distributed in a controlled manner that is customized to the needs of the patient, this innovation not only expedites the formulation process but also enhances therapeutic outcomes.

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[48] Figure 3: https://www.linkedin.com/pulse/pharmaceutical-artificial-intelligence-2020-sector-heating-buvailo?utm_source=share&utm_medium=member_android&utm_campaign=share_via