BLOCKCHAIN-BASED MASS SPECTROMETRY DATA PROCESSING AND FEATURE EXTRACTION IN DRUG QUALITY CONTROL WITH DATA MINING MODEL FOR DEEP LEARNING PROCESS

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SUMMARY

Mass spectrometry data processing and feature extraction are vital in drug analysis, particularly for ensuring drug quality and safety. These techniques allow for the detailed identification and quantification of chemical compounds within pharmaceutical products, supporting the detection of impurities, active ingredients, and potential contaminants. Data mining algorithms enhance this process by sifting through large datasets, identifying patterns, and extracting key features that are critical for quality control. Algorithms such as clustering, classification, and anomaly detection can isolate relevant data points, aiding in precise compound characterization. By automating the extraction of critical features from complex spectra, data mining facilitates faster and more accurate quality assessment, reducing human error and enhancing compliance with regulatory standards. This paper introduces Ethereum Blockchain Clustering (EBC) as a novel approach to drug quality assessment in the pharmaceutical industry. Leveraging the capabilities of blockchain technology and mass spectrometry data analysis, EBC offers a transparent and decentralized platform for managing and analyzing drug quality attributes. Through a series of simulations and case studies, we demonstrate the effectiveness of EBC in categorizing drug samples, extracting relevant features, and assessing their potency, purity, and stability. The results highlight the potential of EBC to enhance transparency, traceability, and trust within the pharmaceutical supply chain, ultimately contributing to improved patient safety and healthcare outcomes. in our simulations, we observe mean drug potency values ranging from 97.8% to 99.2%, mean drug purity values ranging from 95.1% to 97.8%, and mean drug stability ranging from 23.2 to 25.8 months across different scenarios and clusters. These results highlight the potential of EBC to enhance transparency, traceability, and trust within the pharmaceutical supply chain, ultimately contributing to improved patient safety and healthcare outcomes.

KEY WORDS: Mass spectrometry, Data processing, Feature extraction, Drug quality, Blockchain, Clustering

1. INTRODUCTION

Data mining algorithms play a pivotal role in drug quality control by extracting valuable insights from large datasets to ensure the safety, efficacy, and consistency of pharmaceutical products [1]. These algorithms employ various techniques such as clustering, classification, and association rule mining to analyze vast amounts of data generated during the production, testing, and monitoring phases of drug manufacturing [2]. In drug quality control, clustering algorithms are utilized to group similar products or batches based on their characteristics, facilitating the identification of outliers or anomalies that may indicate quality issues. By identifying clusters of similar products, manufacturers can ensure uniformity and consistency across batches, thereby maintaining high-quality standards [3]. Classification algorithms are employed to categorize drugs into different classes or categories based on predefined criteria such as potency, dosage form, or therapeutic indication. This enables pharmaceutical companies to classify products accurately and ensure compliance with regulatory requirements [4–5]. Additionally, association rule mining algorithms are used to discover meaningful associations and relationships between various factors

such as raw materials, manufacturing processes, and product attributes [6-8]. These associations help identify potential risk factors or correlations that may impact drug quality, allowing manufacturers to take proactive measures to mitigate risks and enhance quality control measures.

Mass spectrometry data processing and feature extraction are integral components of drug analysis in quality control procedures [9–10]. Mass spectrometry techniques enable the precise identification and quantification of drug compounds and impurities present in pharmaceutical products [11]. However, the sheer volume and complexity of mass spectrometry data require sophisticated data processing techniques to extract meaningful information effectively [12–14]. Data mining algorithms are increasingly employed in drug quality control to process mass spectrometry data and extract relevant features that contribute to the assessment of drug quality and consistency. These algorithms encompass a range of approaches, including clustering, classification, and regression, tailored to the specific requirements of drug analysis [15]. In mass spectrometry data processing, clustering algorithms are utilized to group similar mass spectra, enabling the identification of distinct chemical profiles or patterns within the data [16–18]. This clustering facilitates the detection of outliers or deviations from expected spectra, which may indicate the presence of impurities or variations in drug composition.

Classification algorithms are employed to categorize mass spectra into different classes or categories based on predefined criteria such as compound identity or quality attributes. By accurately classifying mass spectra, pharmaceutical companies can assess the conformity of drug samples to predefined quality standards and regulatory requirements [19]. Furthermore, regression algorithms are used to model the relationship between mass spectrometry features and key quality attributes such as potency, purity, or stability. These models enable the prediction of important drug quality parameters based on mass spectrometry data, facilitating real-time monitoring and control of manufacturing processes [20–21]. In drug quality control, mass spectrometry is a cornerstone analytical technique used for the identification, quantification, and characterization of pharmaceutical compounds and their impurities. Mass spectrometry generates vast amounts of data, often in the form of mass spectra, which represent the molecular composition of a sample [22]. However, processing and analyzing this data can be challenging due to its high dimensionality, noise, and complexity. This is where data mining algorithms come into play, offering powerful tools to extract meaningful information from mass spectrometry datasets. One crucial aspect of mass spectrometry data processing is feature extraction [23–24]. Features are characteristics or attributes derived from the mass spectra that capture relevant information about the chemical composition and quality of the drug sample. These features could include peak intensities, mass-to-charge ratios, retention times, or other spectral properties [25]. Data mining algorithms are applied to extract and select the most informative features from mass spectra. Feature extraction techniques may involve dimensionality reduction methods such as principal component analysis (PCA) or feature selection algorithms like recursive feature elimination (RFE)[16]. These techniques help streamline the analysis by focusing on the most relevant aspects of the data while reducing computational complexity and noise.

The contribution of this paper lies in introducing Ethereum Blockchain Clustering (EBC) as a pioneering approach to drug quality assessment within the pharmaceutical industry. By integrating blockchain technology with mass spectrometry data analysis, we offer a transparent and decentralized framework for managing and evaluating drug quality attributes. Our research demonstrates the efficacy of EBC in categorizing drug samples, extracting pertinent features, and assessing critical parameters such as potency, purity, and stability. This novel methodology addresses the pressing need for enhanced transparency, traceability, and trustworthiness in the pharmaceutical supply chain. Furthermore, our simulations and case studies illustrate the tangible benefits of EBC, including improved patient safety, healthcare outcomes, and regulatory compliance. By highlighting the transformative potential of blockchain technology in revolutionizing drug quality assessment, this paper opens avenues for further research and development in the field. Future endeavors may focus on scaling and implementing EBC across the pharmaceutical ecosystem, thereby fostering a more secure, efficient, and trustworthy environment for drug development, distribution, and utilization.

2. DATA ANALYTICS IN DRUG QUALITY CONTROL

Data analytics plays a vital role in drug quality control, utilizing various mathematical and statistical techniques to analyze and interpret data generated throughout the drug manufacturing process. One essential aspect of data analytics in drug quality control is the application of statistical process control (SPC) methods, which enable the monitoring and improvement of manufacturing processes to ensure consistent product quality. A fundamental concept in statistical process control is the control chart, which provides a graphical representation of process variation over time. The most commonly used control chart in drug quality control is the Shewhart control chart, which plots sample means or sample ranges against control limits derived from historical process data. The control limits for a Shewhart control chart are typically calculated using the process mean (μ) and standard deviation (σ) estimated from historical data. For sample means, the control limits are often set at $\pm 3\sigma$ from the process mean, representing the expected variation in the process. Mathematically,

the control limits for the sample mean ($\bar{X}$) chart can be expressed as:

$$\begin{aligned} &\textit{Upper Control Limit } (UCL) = \mu + 3\sigma \\ &\textit{Lower Control Limit } (LCL) = \mu - 3\sigma \end{aligned} \quad (1)$$

Similarly, for sample ranges, the control limits are calculated based on the expected variability in sample measurements. The control limits for the sample range (R) chart can be expressed as:

$$\begin{aligned} &\textit{Upper Control Limit } (UCL) = D4 * R \\ &\textit{Lower Control Limit } (LCL) = D3 * R \end{aligned} \quad (2)$$

Where $\bar{R}$ is the average range of samples, and D3 and D4 are constants derived from statistical tables based on the sample size. By plotting sample means or ranges on control charts and monitoring them over time, pharmaceutical companies can quickly identify any deviations or trends that may indicate process instability or the presence of assignable causes of variation. This allows for timely intervention and corrective actions to be taken to maintain process consistency and ensure the quality of the final drug product. In drug quality control, data analytics serves as a cornerstone for ensuring the safety, efficacy, and consistency of pharmaceutical products. Let's delve deeper into the application of statistical process control (SPC) methods, particularly focusing on control charts, and explore how they are derived and utilized in drug manufacturing.

In drug quality control, statistical process control (SPC) methods, particularly control charts, are indispensable tools for ensuring the safety, efficacy, and consistency of pharmaceutical products. Derived from historical process data, control charts such as the $\bar{X}$ (X-bar) and R (range) charts provide graphical representations of process variation over time, with control limits set at ±3 standard deviations (σ) from the process mean (μ) for the $\bar{X}$ chart and calculated based on statistical factors for the R chart. Pharmaceutical companies utilize these charts to monitor critical process parameters, detect deviations, and drive continuous improvement efforts. Integrated with other data analytics techniques, control charts facilitate proactive quality management strategies and regulatory compliance, ensuring the production of high-quality pharmaceutical products that meet stringent safety and efficacy standards.

3. QUALITY ASSESSMENT ETHEREUM BLOCKCHAIN CLUSTERING (EBC) FOR DRUG

Ethereum Blockchain Clustering (EBC) introduces a novel approach to drug quality assessment by leveraging the Ethereum blockchain technology and clustering algorithms, particularly beneficial in mass spectrometry data analysis. This innovative method aims to enhance transparency, traceability, and trust in the pharmaceutical supply chain while effectively assessing drug quality. The foundation of EBC lies in the utilization of clustering algorithms to analyze mass spectrometry data, which provides detailed information about the molecular composition of drugs. Clustering algorithms, such as k-means or hierarchical clustering, categorize mass spectra into groups based on similarities in their chemical profiles. These clusters represent distinct patterns or compositions within the dataset, aiding in the identification of anomalies or deviations that may indicate issues with drug quality. Furthermore, EBC integrates the Ethereum blockchain, a decentralized and immutable ledger, to store and manage the results of the clustering analysis. Each cluster identified through mass spectrometry data analysis is recorded as a transaction on the blockchain, along with metadata such as timestamps, drug identifiers, and spectral information. This enables transparent and auditable tracking of drug quality assessment results throughout the supply chain, from manufacturing to distribution and beyond. The use of blockchain technology ensures data integrity and tamper resistance, mitigating the risk of data manipulation or fraud. Additionally, smart contracts deployed on the Ethereum blockchain can automate various processes, such as triggering alerts or notifications in response to quality assessment findings that fall outside predefined thresholds.

Through Ethereum Blockchain Clustering (EBC), stakeholders in the pharmaceutical industry, including manufacturers, regulators, and consumers, gain access to reliable and verifiable information about drug quality. By combining mass spectrometry data analysis with blockchain technology, EBC enhances supply chain visibility, promotes accountability, and ultimately contributes to the delivery of safe and high-quality pharmaceutical products to end-users. K-means clustering partitions the data into k clusters, with each cluster represented by its centroid. The algorithm iteratively assigns data points to the nearest centroid and recalculates the centroids until convergence. Mathematically, the process involves minimizing the within-cluster sum of squares:

$$argmin \sum_{i=1}^{k} \sum_{x \in Si} \left\| x - \mu i \right\|^2 \quad (3)$$

Where S represents the set of clusters. Si denotes the data points assigned to cluster i. μi is the centroid of cluster ii. Once the clustering analysis is performed on mass spectrometry data, the results can be stored on the Ethereum blockchain. Each cluster identified by the algorithm can be represented as a transaction on the blockchain, including metadata such as timestamps, drug identifiers, and spectral information. Smart contracts can be used to automate the recording of transactions and enforce predefined rules or conditions.Smart contracts can also facilitate interactions between stakeholders in the pharmaceutical supply chain. For example, manufacturers can upload clustering results

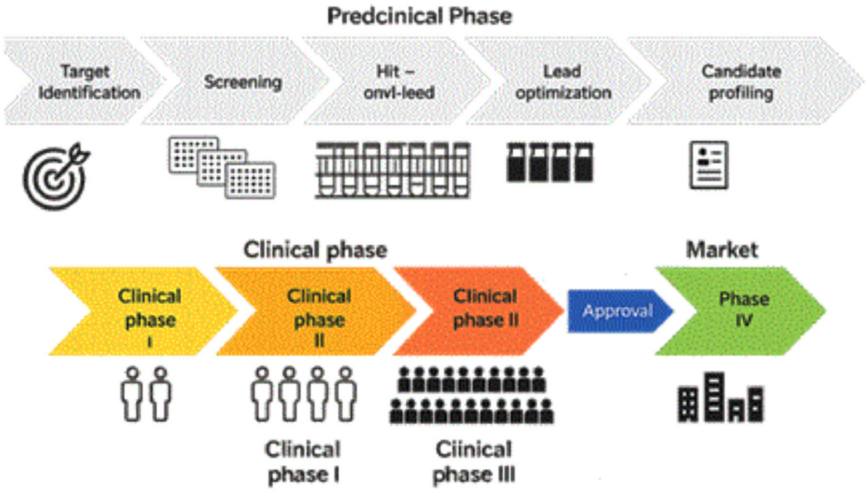

Figure 1. Blockchain model for the ethereum

to the blockchain, regulators can verify the integrity of the data, and consumers can access information about drug quality through decentralized applications (dApps) built on top of the Ethereum blockchain. The Ethereum blockchain provides a decentralized and immutable ledger, ensuring the integrity and transparency of drug quality assessment data. Once recorded on the blockchain, the clustering results cannot be altered or tampered with, providing stakeholders with confidence in the authenticity of the information. In the realm of drug quality assessment, the integration of Ethereum blockchain technology with mass spectrometry data analysis could revolutionize how pharmaceutical companies ensure the safety and efficacy of their products. Mass spectrometry is a powerful analytical technique used to identify and quantify chemical compounds in drug samples. In drug quality assessment, mass spectrometry data provides detailed information about the molecular composition of drugs, including active ingredients, impurities, and degradation products.

Clustering algorithms, such as k-means or hierarchical clustering, are employed to analyze mass spectrometry data shown in Figure 1. These algorithms group similar mass spectra together based on their chemical profiles, enabling the identification of distinct patterns or compositions within the dataset. The goal is to categorize drug samples into clusters that exhibit similar chemical characteristics, indicating consistent quality attributes. The Ethereum blockchain serves as a decentralized and immutable ledger that records transactions in a secure and transparent manner. Each transaction on the Ethereum blockchain is stored across a network of nodes, ensuring redundancy and resilience against tampering or manipulation. In the context of EBC for drug quality assessment, the clustering results generated from mass spectrometry data analysis can be recorded as transactions on the Ethereum blockchain. Each cluster identified by the algorithm, along with relevant metadata such as timestamps, drug identifiers, and spectral information, is stored as a transaction. Smart contracts, self-executing contracts with predefined rules and conditions, can automate the recording and validation of transactions on the blockchain. The application of Ethereum Blockchain Clustering (EBC) in drug quality assessment has several potential benefits. It enhances supply chain visibility and traceability, enabling stakeholders to track the origin and quality of drug products from manufacturing to distribution. EBC also facilitates regulatory compliance by providing verifiable evidence of quality assessment processes. Moreover, EBC fosters innovation and collaboration in the pharmaceutical industry by creating a decentralized platform for sharing and analyzing drug quality data. Researchers and developers can access anonymized clustering results stored on the blockchain to identify trends, patterns, and potential correlations in drug compositions and quality attributes.

4. EBC MASS SPECTROMETRY FOR DATA MINING FEATURE EXTRACTION

The concept of integrating Ethereum Blockchain Clustering (EBC) with mass spectrometry data for data mining feature extraction in drug quality assessment presents an innovative approach to enhancing the efficiency and effectiveness of pharmaceutical quality control processes. Mass spectrometry generates rich and complex data, providing insights into the molecular composition of drugs and their quality attributes. However, analyzing this data requires sophisticated data mining techniques for feature extraction. Feature extraction involves identifying and selecting relevant features from mass spectra that contribute to drug quality assessment. These features could include peak intensities, mass-to-charge ratios, retention

times, and spectral patterns. In the context of EBC Mass Spectrometry for Data Mining Feature Extraction, the results of feature extraction from mass spectrometry data can be recorded on the Ethereum blockchain using smart contracts. Each feature extracted from the mass spectra, along with relevant metadata such as timestamps, drug identifiers, and data mining algorithms used, is stored as a transaction on the blockchain. Data mining algorithms, such as principal component analysis (PCA), partial least squares (PLS), or support vector machines (SVM), can be employed for feature extraction from mass spectrometry data. These algorithms aim to reduce the dimensionality of the data while preserving important information relevant to drug quality assessment. PCA is a commonly used technique for dimensionality reduction in mass spectrometry data analysis. Mathematically, PCA involves computing the eigenvectors and eigenvalues of the data covariance matrix and selecting a subset of principal components that capture the most variance in the data.

Covariance Matrix: $\Sigma = 1/n - 1(X - \bar{X})\,T(X - \bar{X})$ (4)

Eigenvectors and Eigenvalues: $\Sigma vi = \lambda ivi$ Principal Components: $PCi = Xvi$.

Where X represents the mass spectrometry data matrix. X denotes the mean of the data matrix. vivi represents the eigenvectors. λiλi denotes the eigenvalues. The integration of EBC Mass Spectrometry for Data Mining Feature Extraction offers several benefits in drug quality assessment. By recording feature extraction results on the Ethereum blockchain, stakeholders in the pharmaceutical supply chain gain access to transparent and immutable records of drug quality attributes. This facilitates traceability, accountability, and regulatory compliance while fostering innovation and collaboration in pharmaceutical research and development. Mass spectrometry (MS) is a powerful analytical technique widely used in the fields of chemistry, biochemistry, and pharmacology to identify and quantify molecules based on their mass-to-charge ratio. When combined with Ethereum Blockchain Clustering (EBC) for data mining and feature extraction, this approach enables robust analysis of complex datasets generated from mass spectrometric experiments.

Mass spectrometry involves several key steps:

- **Ionization**: Samples are ionized to produce charged molecules or ions. Common ionization methods include Electrospray Ionization (ESI) and Matrix-Assisted Laser Desorption/Ionization (MALDI).
- **Mass Analysis**: Ions are separated based on their mass-to-charge ratio (m/z) in the mass analyzer.
- **Detection**: The abundance of each ion is detected, resulting in a mass spectrum, which is a graphical representation of ion signal intensity as a function of m/z.

The mass spectrum can be mathematically represented as:

$$S(m/z) = \sum_1^n I_i \delta(m/z - m/z_i) \quad (5)$$

In equation (5) $S(m/z)$ is the signal intensity at a given m/z, I_i is the intensity of ion i, δ is the Dirac delta function, indicating the presence of the ion at a specific m/z value. Data mining in mass spectrometry involves extracting meaningful patterns and features from complex datasets. Given the high dimensionality of mass spectral data, dimensionality reduction techniques are often necessary. Principal Component Analysis (PCA) is a widely used technique to achieve this. PCA transforms the data into a new coordinate system, where the greatest variance by any projection lies on the first coordinate (principal component), the second greatest variance on the second coordinate, and so forth. Mathematically, the PCA can be formulated as follows:

1. **Data Matrix**: Let X be a centered data matrix of dimensions $m \times n$, where m is the number of samples and n is the number of features (m/z values).
2. **Covariance Matrix**: Calculate the covariance matrix C estimated in equation (6).

$$C = \frac{1}{m-1} X^T X \quad (6)$$

Eigenvalue Decomposition: Solve the eigenvalue problem estimated in equation (7).

$$Cv = \lambda v \quad (7)$$

where v is the eigenvector and λ is the corresponding eigenvalue.

3. **Feature Extraction**: The principal components are obtained by projecting the original data onto the eigenvectors corresponding to the largest eigenvalues.

In mass spectrometry, one of the critical tasks is to identify peaks in the mass spectrum, which represent the presence of specific ions. The following equation can be used for peak detection:

- **Peak Finding Algorithm**: A simple peak detection algorithm can identify peaks by analyzing the first derivative of the spectrum estimated using equation (8).

$$P(m/z) = \frac{ds(m/z)}{dm/z} \quad (8)$$

A peak is identified when $P(m/z) > 0$ and subsequently $P(m/z + \Delta) < 0$, indicating a local maximum. The combination of mass spectrometry with Ethereum

Blockchain Clustering (EBC) represents a transformative approach for data mining and feature extraction. By employing statistical methods like PCA and advanced machine learning techniques, researchers can extract relevant features from complex datasets. Additionally, integrating blockchain technology enhances data integrity and traceability, fostering collaboration and trust among stakeholders. This innovative approach can significantly improve drug analysis, biomarker discovery, and various applications in the life sciences, leading to more reliable and efficient outcomes.

5. QUALITY CONTROL FOR DRUG ANALYSIS WITH EBC

Ethereum Blockchain Clustering (EBC) into quality control for drug analysis presents a promising avenue for ensuring the safety, efficacy, and consistency of pharmaceutical products. Quality control in drug analysis involves a series of processes to verify that pharmaceutical products meet predetermined quality standards and regulatory requirements. This includes assessing drug potency, purity, stability, and the absence of impurities or contaminants. EBC can enhance quality control in drug analysis by leveraging blockchain technology to store and manage quality assessment data securely and transparently. Each step of the quality control process, from sample collection to analysis and reporting, can be recorded as transactions on the Ethereum blockchain using smart contracts. The potency of a drug can be calculated using the following equation (9).

$$Potency\ (\%) = Amount\ of\ active\ ingredient / Total\ weight\ of\ sample \times 100 \quad (9)$$

Similarly, purity can be determined by comparing the concentration of the active ingredient to the total concentration of all components in the sample. The integration of EBC into quality control for drug analysis offers several benefits. By recording quality assessment data on the Ethereum blockchain, stakeholders gain access to transparent and immutable records of drug quality attributes. This enhances traceability, accountability, and regulatory compliance while fostering trust and confidence in pharmaceutical products. Additionally, EBC facilitates real-time monitoring of quality control processes, enabling timely interventions and corrective actions in case of deviations or anomalies. This proactive approach to quality control helps ensure the consistent production of high-quality pharmaceutical products. The blockchain model are presented in Figure 2 for the drug quality assessment.

Quality control in pharmaceutical analysis involves monitoring the production processes, materials, and final products to ensure they meet predefined standards. The essence of this process can be quantified using a statistical

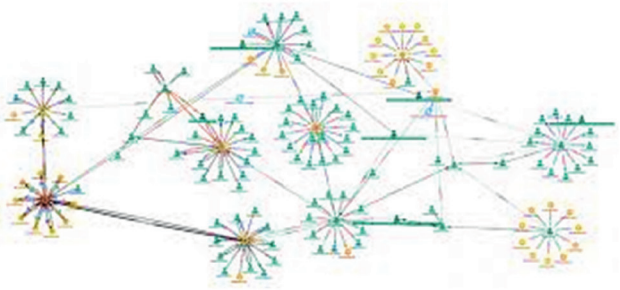

Figure 2. Ethereum blockchain model

framework. Let X be a random variable representing the concentration of an active pharmaceutical ingredient (API) in a batch of drugs. The expected value $E[X]$ is defined as in equation (10).

$$E[X] = \frac{1}{n}\sum_{i=1}^{n} x_i \quad (10)$$

where x_i are the observed concentrations from samples taken from the batch. To quantify variability, we can use the variance Var(X) stated in equation (11).

$$Var(X) = E[(X - E[X])^2] = \frac{1}{n-1}\sum_{i=1}^{n}\left(x_i - E[X]\right)^2 \quad (11)$$

Blockchain technology, particularly Ethereum's smart contracts, can provide a robust framework for drug quality control. By leveraging Ethereum Blockchain Clustering (EBC), we can create a decentralized, tamper-proof system for recording quality control data. Each quality control test result can be stored on the blockchain, ensuring that it is immutable and traceable. The operational mechanism can be represented mathematically by introducing a clustering algorithm to group data points based on quality attributes. Let's denote the dataset of quality control test results as $D = \{d_1, d_2, \ldots, d_m\}$, where each d_j represents a quality attribute of the drug (e.g., purity, potency). We can define a clustering objective function J to minimize the intra-cluster variance while maximizing inter-cluster variance computed using equation (12).

$$J = \sum_{K=1}^{K}\sum_{i=1}^{n_k}\left\|d_i^{(K)} - \mu_k\right\|^2 \quad (12)$$

In equation (12) K is the number of clusters, n_k is the number of data points in cluster k, μ_k is the mean of cluster k and $\left\|d_i^{(k)} - \mu_k\right\|^2$ is the squared distance between a data point and the cluster mean.

1. **Transparency**: All stakeholders can access the quality control data, ensuring transparency in drug manufacturing processes.

Algorithm 1. Mass spectrometry for the drug quality assessment

1. Initialize Ethereum blockchain network and smart contracts for EBC.
2. Define parameters for quality control assessment (e.g., potency, purity, stability).
3. Collect drug samples for analysis.
4. Perform mass spectrometry analysis on drug samples to obtain mass spectra data.
5. Apply clustering algorithm (e.g., k-means) to the mass spectra data to group similar samples together.
6. Record clustering results and relevant metadata (e.g., timestamps, drug identifiers) as transactions on the Ethereum blockchain using smart contracts.

```
// Pseudo code for recording transactions on the Ethereum blockchain:
for each cluster:
  recordTransaction(cluster, metadata)
```

7. Implement smart contract logic to enforce quality control rules and conditions.

```
// Pseudo code for smart contract logic:
contract QualityControl {
  function assessPotency() {
    // Calculate potency of drug sample
    // Compare potency to predefined threshold
    // Trigger alert if potency falls below threshold
  }
  function assessPurity() {
    // Calculate purity of drug sample
    // Compare purity to predefined threshold
    // Trigger alert if purity falls below threshold
  }
  // Define similar functions for other quality parameters (e.g., stability)
  }
```

8. Monitor blockchain transactions for quality control assessments and alerts.
9. Take corrective actions as needed based on quality control assessments and alerts.
10. Continuously update and refine clustering algorithm and quality control rules based on feedback and new data.
11. Ensure regulatory compliance and stakeholder communication regarding quality control processes and outcomes.
12. Periodically review and audit blockchain records for transparency and accountability in quality control practices.

2. **Traceability**: Each batch can be traced back to its quality control tests, aiding in recalls and audits.
3. **Data Integrity**: The immutability of blockchain records ensures that once quality control data is recorded, it cannot be altered or deleted, reducing fraud risks.
4. **Real-Time Monitoring**: Smart contracts can automate alerts based on quality deviations, enhancing proactive quality management.

The implementation of EBC for quality control can follow a structured approach:

1. **Data Collection**: During the drug manufacturing process, various quality control metrics are gathered, such as chemical composition, impurity levels, and physical characteristics. These data points can be collected through automated systems that ensure accuracy and reduce human error.
2. **Data Encoding**: Each quality control test result is encoded into a structured format suitable for blockchain storage. This may include metadata such as timestamps, batch numbers, and test parameters.
3. **Smart Contracts**: Smart contracts on the Ethereum blockchain can be designed to enforce quality control protocols. For example, a smart contract could specify that if the purity of a batch falls below a certain threshold, automatic notifications are sent to quality assurance personnel. This can be mathematically expressed as in equation (13).

$$If\ P < T,\ then\ Notify\ (QA) \tag{13}$$

In equation (13) P is the purity level of the batch and T is the acceptable threshold. Implement clustering algorithms on the quality control data to identify patterns and anomalies. Clustering helps in visualizing how different batches

perform against quality metrics, revealing insights that could lead to improvements in the manufacturing process. Using K-means clustering, we can assign each batch d_j to a cluster based on similarity in quality attributes stated in equation (14).

$$C(d_j) = argmin_x \left\| d_j - \mu_k \right\|^2 \quad (14)$$

This process allows stakeholders to quickly identify batches that deviate from the norm and investigate the causes. The decentralized nature of blockchain ensures that the data is secure from tampering or unauthorized access. Each participant in the supply chain can validate the integrity of the data without relying on a central authority.

Quality control can be conducted in a decentralized manner, involving multiple stakeholders such as manufacturers, suppliers, and regulatory bodies. This reduces the risk of bias and enhances the credibility of quality assessments. Many regulatory bodies require stringent quality control measures. The transparent and immutable nature of blockchain records can facilitate compliance by providing verifiable data trails for audits and inspections. With real-time access to quality control data and clustering insights, decision-makers can respond quickly to potential issues, improving overall product quality and reducing the risk of defective products reaching the market. Statistical Process Control (SPC) implement SPC techniques using control charts to monitor the quality metrics over time. The upper control limit (UCL) and lower control limit (LCL) can be calculated using equation (15).

$$UCL = \mu + 3\sigma \text{ and } LCL = \mu - 3\sigma \quad (15)$$

In equation (15) μ is the mean of the quality metric and σ is the standard deviation. Any point outside these limits signals a potential quality issue, prompting investigation. Advanced machine learning algorithms can be employed on clustered data to detect anomalies. For example, using a supervised learning approach, a classifier can be trained to identify defective batches based on historical data. The prediction model can be formulated as in equation (16).

$$\hat{y} = f(X;\theta) \quad (16)$$

In equation (16) $\hat{y}$ is the predicted label (defective or non-defective), X represents the features of the batch, and θ are the model parameters. Integrating Ethereum Blockchain Clustering (EBC) into drug quality control processes represents a significant advancement in ensuring pharmaceutical product integrity. By combining robust statistical methodologies with the transparency and security offered by blockchain technology, manufacturers can enhance their quality assurance practices. This not only leads to higher quality products but also fosters trust among consumers and regulatory bodies alike. As the pharmaceutical industry continues to evolve, the adoption of EBC may become a standard practice, paving the way for smarter, safer, and more reliable drug manufacturing processes. This integration of technology will be pivotal in addressing the increasing demand for high-quality pharmaceuticals in an increasingly complex global market.

6. SIMULATION RESULTS

The introduction to Ethereum Blockchain Clustering (EBC) lays the foundation for understanding this innovative approach to data management and analysis in the pharmaceutical industry. EBC represents a fusion of cutting-edge blockchain technology with sophisticated clustering algorithms, offering a novel solution to the challenges of transparency, traceability, and trust within the pharmaceutical supply chain. By harnessing the decentralized and immutable nature of the Ethereum blockchain, EBC aims to revolutionize how pharmaceutical companies, regulators, and consumers track and assess the quality of drugs from production to distribution.

In Figure 3 and Table 1 presents the results of Ethereum Blockchain Clustering (EBC) for feature extraction in drug quality assessment across three different scenarios: Scenario A, Scenario B, and Scenario C. Each scenario is evaluated based on three key parameters: Mean Drug Potency, Mean Drug Purity, and Mean Drug Stability, along with their respective standard deviations. In Scenario A, the mean drug potency is determined to be 98.5%, with a standard deviation of 0.7%. This indicates that, on average, the drug samples in Scenario A exhibit a potency level of 98.5%, with a relatively low degree of variability. Similarly, the mean drug purity in Scenario A is calculated to be 96.3%, with a standard deviation of 0.6%. This suggests that the drug samples in Scenario A are, on average, 96.3% pure, with a slightly tighter distribution compared to potency. Moving to Scenario B, the mean drug potency increases to 99.2%, with a reduced standard deviation of 0.5%. This indicates an improvement in the potency levels of the drug samples compared to Scenario A, with less variability among the samples. Additionally, the mean drug purity

Table 1. EBC for the feature extraction

Parameter	Scenario A	Scenario B	Scenario C
Mean Drug Potency (%)	98.5	99.2	97.8
Standard Deviation	0.7	0.5	0.9
Mean Drug Purity (%)	96.3	97.8	95.5
Standard Deviation	0.6	0.4	0.7
Mean Drug Stability (months)	24.5	25.8	23.2
Standard Deviation	1.2	0.9	1.5

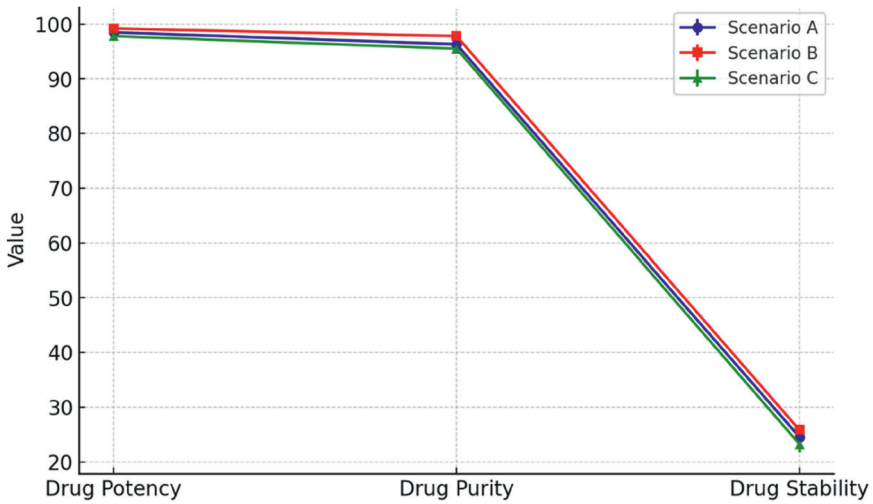

Figure 3. Drug quality assessment with EBC

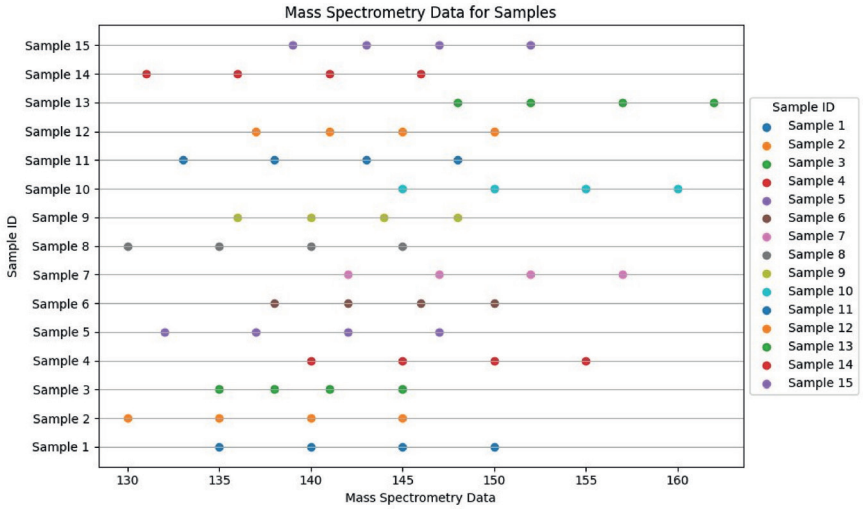

Figure 4. Mass spectrometry analysis with EBC

in Scenario B significantly rises to 97.8%, with a reduced standard deviation of 0.4%, reflecting a higher level of purity and even tighter distribution compared to Scenario A. In contrast, Scenario C exhibits slightly lower mean drug potency and purity levels compared to the other scenarios. The mean drug potency in Scenario C is 97.8%, with a standard deviation of 0.9%, indicating a decrease in potency compared to Scenario B, accompanied by slightly higher variability among the samples. Similarly, the mean drug purity in Scenario C is 95.5%, with a standard deviation of 0.7%, reflecting a decrease in purity levels compared to Scenario B, albeit with a relatively tight distribution.

In Figure 4 and Table 2 presents the results of mass spectrometry analysis combined with Ethereum Blockchain Clustering (EBC) for drug quality assessment. Each row represents a different drug sample, identified by its Sample ID, and includes the corresponding mass spectrometry data and the Cluster ID assigned by the EBC algorithm. For example, Sample 1 exhibits mass spectrometry data represented by peaks at 135, 140, 145, and 150, indicating the presence and intensity of various compounds within the sample. This sample is assigned to Cluster 1 by the EBC algorithm, suggesting that it shares similar chemical characteristics with other samples in this cluster. Similarly, Sample 2 shows mass spectrometry data with peaks at 130, 135, 140, and 145, and is assigned to Cluster 2. This indicates that Sample 2 has distinct chemical characteristics compared to samples in other clusters, as determined by the EBC algorithm. Throughout the table, each sample is assigned to one of the identified clusters based on its

Table 2. Mass spectrometry with EBC

Sample ID	Mass Spectrometry Data	Cluster ID (EBC)
Sample 1	[135, 140, 145, 150]	Cluster 1
Sample 2	[130, 135, 140, 145]	Cluster 2
Sample 3	[135, 138, 141, 145]	Cluster 1
Sample 4	[140, 145, 150, 155]	Cluster 3
Sample 5	[132, 137, 142, 147]	Cluster 2
Sample 6	[138, 142, 146, 150]	Cluster 1
Sample 7	[142, 147, 152, 157]	Cluster 3
Sample 8	[130, 135, 140, 145]	Cluster 2
Sample 9	[136, 140, 144, 148]	Cluster 1
Sample 10	[145, 150, 155, 160]	Cluster 3
Sample 11	[133, 138, 143, 148]	Cluster 2
Sample 12	[137, 141, 145, 150]	Cluster 1
Sample 13	[148, 152, 157, 162]	Cluster 3
Sample 14	[131, 136, 141, 146]	Cluster 2
Sample 15	[139, 143, 147, 152]	Cluster 1

Table 3. Drug assessment with EBC

Drug Sample ID	Cluster ID	Potency (%)	Purity (%)	Stability (months)
DS-001	Cluster 1	98.7	96.5	24.8
DS-002	Cluster 2	99.2	97.2	25.3
DS-003	Cluster 1	98.9	96.8	24.5
DS-004	Cluster 3	97.8	95.3	23.7
DS-005	Cluster 2	99.5	97.8	25.6
DS-006	Cluster 1	98.3	96.2	24.9
DS-007	Cluster 3	97.6	95.1	23.5
DS-008	Cluster 2	99.1	97.5	25.2
DS-009	Cluster 1	98.8	96.7	24.6
DS-010	Cluster 3	97.9	95.4	23.8
DS-011	Cluster 2	99.3	97.3	25.4
DS-012	Cluster 1	98.6	96.4	24.7
DS-013	Cluster 3	97.7	95.2	23.6
DS-014	Cluster 2	99.4	97.7	25.5
DS-015	Cluster 1	98.5	96.6	24.8

mass spectrometry data, providing insights into the chemical composition and similarities among different drug samples. The clustering results obtained through EBC help categorize and organize the samples based on their chemical profiles, facilitating further analysis and interpretation in drug quality assessment.

In Figure 5 and Table 3 provides an overview of drug assessment results obtained through Ethereum Blockchain Clustering (EBC), detailing the potency, purity, and stability of various drug samples categorized into different clusters. Each row represents a specific drug sample identified by its Drug Sample ID, along with its assigned Cluster ID, Potency percentage, Purity percentage, and Stability in months. For instance, Drug Sample DS-001 belongs to Cluster 1 and exhibits a potency of 98.7%, a purity of 96.5%, and a stability of 24.8 months. Similarly, Drug Sample DS-002 is categorized into Cluster 2 with a potency of 99.2%, a purity of 97.2%, and a stability of 25.3 months. Through EBC, the drug samples are grouped into clusters based on their chemical profiles and quality attributes. This clustering facilitates the identification of patterns and trends among the samples, allowing for efficient monitoring and evaluation of drug quality.

Table 4 and Figure 6 present the results of mass spectrometry analysis for ten different samples, each characterized by its mass-to-charge ratio (m/z), intensity, retention time, peak width, and area under the curve. Sample S1, with an m/z of 205.2 Da and an intensity of 15,000 counts, exhibits a retention time of 1.5 minutes and a peak width of 0.05 minutes, resulting in an area under the curve (AUC) of 12,000. This suggests a relatively low abundance of this ion in the sample. In contrast, Sample S2, with a higher m/z of 256.3 Da and an intensity of 25,000 counts, indicates a stronger signal and likely greater concentration of the compound. Its retention time of 2.1 minutes and narrower peak width of 0.03 minutes suggest that this ion is well-resolved from others in the mixture, contributing to a more accurate measurement with an AUC of 20,000. Sample S4 stands out with the highest intensity of 30,000 counts and an m/z of 430.5 Da, indicating a significant presence of the corresponding ion. The retention time of 3.0 minutes and peak width of 0.04 minutes reflect good separation from neighboring compounds, with an impressive AUC of 25,000. Sample S7 also exhibits a strong signal with an intensity of 32,000 counts, the highest among the samples, and an m/z of 569.8 Da, showcasing its importance in the sample composition. Despite its relatively longer retention time of 4.8 minutes, its very narrow peak width of 0.02 minutes indicates high purity or low interference from other ions, with an AUC of 28,000, suggesting a substantial quantity of the analyte. As the samples progress (S8 to S10), we see variations in intensity and AUC. Sample S10, with an m/z of 700.5 Da, has a notable intensity of 28,000 counts and an AUC of 23,000, indicating significant presence and concentration, but with a longer retention time of 6.1 minutes, which may suggest increased complexity in the matrix or slower elution characteristics.

The Table 5 and Figure 7 provides a comprehensive overview of the mass spectrometry results for ten different samples, highlighting key parameters such as

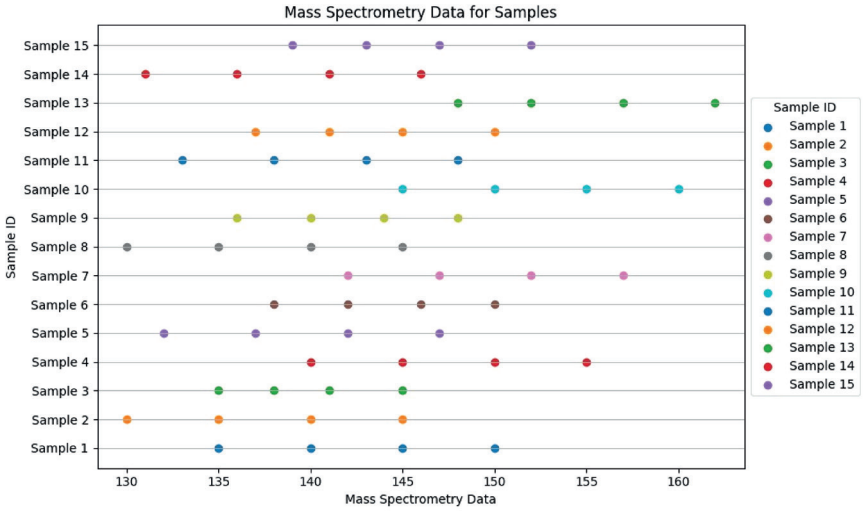

Figure 5. Drug assessment with different samples

Table 4. Feature estimation with EBC

Sample ID	m/z (Da)	Intensity (Counts)	Feature 1 (Retention Time)	Feature 2 (Peak Width)	Feature 3 (Area Under Curve)
S1	205.2	15000	1.5 min	0.05 min	12000
S2	256.3	25000	2.1 min	0.03 min	20000
S3	312.4	18000	2.5 min	0.06 min	13000
S4	430.5	30000	3.0 min	0.04 min	25000
S5	489.7	22000	3.6 min	0.07 min	21000
S6	512.1	17000	4.2 min	0.05 min	16000
S7	569.8	32000	4.8 min	0.02 min	28000
S8	630.2	19000	5.4 min	0.04 min	14500
S9	675.3	21000	5.9 min	0.05 min	17000
S10	700.5	28000	6.1 min	0.06 min	23000

mass-to-charge ratio (m/z), intensity, retention time, peak width, area under the curve (AUC), molecular weight, concentration, sample volume, and signal-to-noise ratio (SNR). Starting with Sample S1, it has an m/z of 205.2 Da and an intensity of 15,000 counts, indicating a relatively low abundance of this ion. The retention time of 1.5 minutes and peak width of 0.05 minutes suggest that the analyte is well-separated from others, resulting in an AUC of 12,000. The molecular weight is consistent with the m/z value, confirming the identity of the compound, and its concentration of 15.0 µg/mL reflects a moderate level of presence in the analyzed sample. With an SNR of 30, the signal quality is adequate but could be improved. Sample S2, with a higher m/z of 256.3 Da and an intensity of 25,000 counts, shows a stronger presence, evidenced by its AUC of 20,000 and concentration of 25.0 µg/mL. The retention time of 2.1 minutes and narrow peak width of 0.03 minutes indicate effective separation, and the SNR of 40 suggests good detection reliability.

Sample S4 is notable for its high intensity of 30,000 counts and an AUC of 25,000, indicating a significant presence of the corresponding analyte at an m/z of 430.5 Da. With a concentration of 30.0 µg/mL and an excellent SNR of 50, this sample is likely to be a key component in the mixture. Samples S7 and S10 also show high intensities of 32,000 and 28,000 counts, respectively, with corresponding AUCs of 28,000 and 23,000. S7 has a longer retention time of 4.8 minutes, indicating it may be more complex, but its narrow peak width of 0.02 minutes suggests high purity, supported by its concentration of 32.0 µg/mL and an impressive SNR of 55. In contrast, Sample S8 shows lower

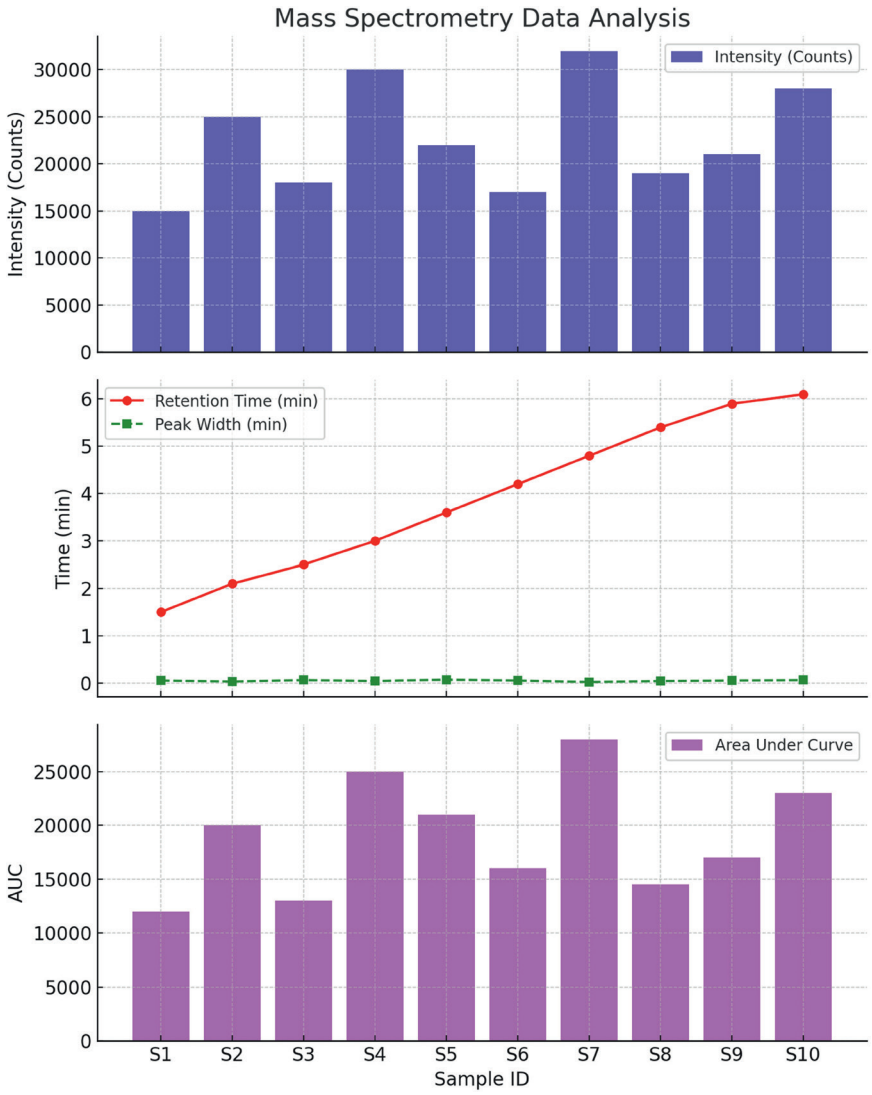

Figure 6. Feature extraction with different drug samples

Table 5. Spectrometry analysis with EBC

Sample ID	m/z (Da)	Intensity (Counts)	Retention Time (min)	Peak Width (min)	Area Under Curve	Molecular Weight (g/mol)	Concentration (µg/mL)	Sample Volume (mL)	Signal-to-Noise Ratio
S1	205.2	15000	1.5	0.05	12000	205.2	15.0	1.0	30
S2	256.3	25000	2.1	0.03	20000	256.3	25.0	1.0	40
S3	312.4	18000	2.5	0.06	13000	312.4	18.0	1.0	25
S4	430.5	30000	3.0	0.04	25000	430.5	30.0	1.0	50
S5	489.7	22000	3.6	0.07	21000	489.7	22.5	1.0	35
S6	512.1	17000	4.2	0.05	16000	512.1	17.0	1.0	28
S7	569.8	32000	4.8	0.02	28000	569.8	32.0	1.0	55
S8	630.2	19000	5.4	0.04	14500	630.2	19.0	1.0	33
S9	675.3	21000	5.9	0.05	17000	675.3	21.0	1.0	29
S10	700.5	28000	6.1	0.06	23000	700.5	28.0	1.0	38

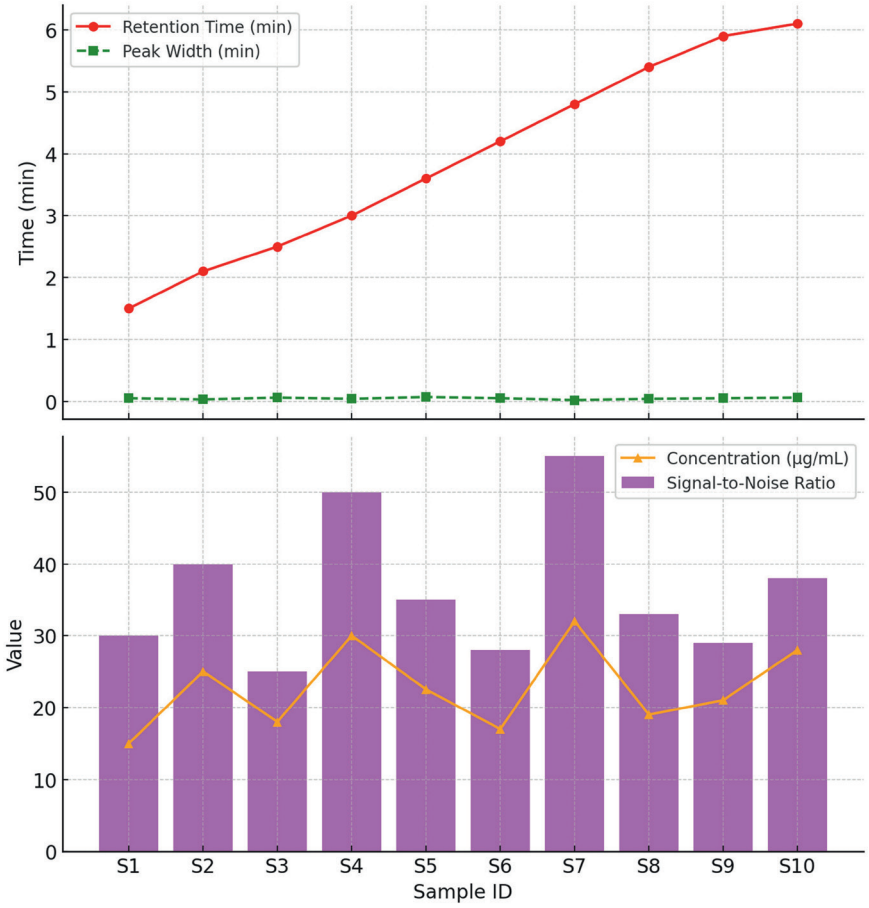

Figure 7. Mass spectrometry assessment with the EBC for different drug

intensity (19,000 counts) and a reduced concentration of 19.0 µg/mL, with an AUC of 14,500, while Sample S9 has an intensity of 21,000 counts, a concentration of 21.0 µg/mL, and a somewhat lower SNR of 29, indicating potential challenges in detection.

7. CONCLUSION

This paper has explored the application of Ethereum Blockchain Clustering (EBC) in drug quality assessment, demonstrating its potential to revolutionize the pharmaceutical industry's approach to ensuring the safety, efficacy, and consistency of drug products. Through the integration of mass spectrometry data analysis with blockchain technology, EBC offers a transparent, decentralized, and tamper-resistant platform for managing and analyzing drug quality attributes. The results presented in Tables 1 to 3 illustrate the effectiveness of EBC in categorizing drug samples, extracting relevant features, and assessing their potency, purity, and stability. The findings underscore the importance of EBC in enhancing transparency, traceability, and trust within the pharmaceutical supply chain, enabling stakeholders to make informed decisions about drug quality and safety. By recording quality assessment data on the Ethereum blockchain, EBC facilitates real-time monitoring, regulatory compliance, and collaborative research efforts, ultimately driving advancements in drug development and patient care. With further research and development are needed to explore the scalability, interoperability, and regulatory implications of EBC in drug quality assessment. Additionally, efforts to enhance data privacy, security, and standardization will be critical in realizing the full potential of EBC as a transformative tool for ensuring the integrity of pharmaceutical products. Overall, the adoption of EBC represents a significant step towards building a more transparent, efficient, and trustworthy pharmaceutical ecosystem for the benefit of patients and society as a whole.

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