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Abstract: In order to solve the problems of low accuracy and low efficiency of traditional water quality detection methods, this paper proposed a testing method for pharmaceutical water quality of inorganic hybrid nano drugs. Firstly, the SH-3900A water quality detector was used to collect multiple parameters of pharmaceutical water, and then spectral normalisation analysis was used to classify the collected results. Finally, the spectral difference between qualified samples and abnormal samples was determined by probability evaluation method to achieve the detection of pharmaceutical water quality. Experimental results show that the detection accuracy of this method is up to 95%, and the detection time can be controlled within 15 min. At the same time, the maximum value of stability coefficient is close to 0.8, indicating that the application level of this method is high.

Keywords: inorganic hybrid nano drugs; pharmaceutical water; multiparameter acquisition; quality inspection; sample classification.

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1 Introduction

Water resource used in pharmaceutical process is the most widely used and most used material in pharmaceutical production, and it belongs to a solvent. Pharmaceutical water is the lifeline of the development of pharmaceutical industry, and its quality plays a very important role in drug safety (Dorea, 2019).

With the continuous progress of production technology, pharmaceutical water treatment equipment has been improved to a certain extent, the relevant departments of the state has also made clear the water quality standards. However, due to the difference of water production technology, the quality of pharmaceutical water is also different (Wu et al., 2021). Therefore, it is necessary to study an effective method to detect the quality of pharmaceutical water in order to ensure the safety of drug production (Ding et al., 2019).

In view of the existing problems in the field of pharmaceutical water research, the pharmaceutical water quality detection methods were studied by relevant professional researchers. Lin et al. (2019) proposed a water quality detection method based on UV-Vis absorption spectrum, which solved the problem of spectral data of water quality being easily disturbed by wavelet transform and eliminated noise data in the data. Then, principal component analysis (PCA) is used to reduce the dimension of the data after noise elimination to avoid the over-fitting problem. On this basis, a preprocessing model of water quality spectral data was established based on support vector machine. The model was used to improve the conventional algorithm. Finally, the improved differential evolution algorithm was used to detect water quality. This method can obtain global optimisation in a short time, but the accuracy of water quality detection results is not high, and it is difficult to effectively meet the demand of pharmaceutical water detection. Xue (2019) proposed a multi-parameter detection method for water quality based on random forest classification algorithm. Firstly, the single parameter and multi-parameter related to water quality are fused, and the probability composite matrix of water quality index is obtained by fusion, and the dimension of matrix is reduced. Then, the membership function of water quality fluctuation is obtained by this matrix, and the features with low correlation degree are removed, while the features with high correlation degree are retained. Finally, the features are input into random forest classifier to achieve water quality detection. This method has the advantage of low detection cost, but its performance in detection timeliness needs to be further improved. Yin et al. (2019) proposed a method of abnormal detection of water quality based on supervised learning. In order to achieve baseline correction, this method selects the difference space of samples in different datasets, and then uses orthogonal projection method to eliminate the spectral data in this space. According to the data processing results, the partial least square discriminant method is used to collect the corrected spectral data, forming a new dataset, and then determine the outliers through training. Finally, the abnormal sequence of water quality is obtained by the probability of abnormal water quality, and then the water quality detection is realised. This method can effectively reduce the detection limit of pollutants in water, but it has the problem of poor stability.

In order to improve the quality of inorganic hybrid nano drugs, a new water quality detection method was proposed because of a series of problems existing in the traditional detection methods in water quality detection. The design idea of this method is as follows:

1 Using SH-3900A water quality detector to quickly collect multiple parameters of pharmaceutical water (including pH value, dissolved oxygen, microbial content, conductivity, COD, chroma, turbidity, total organic carbon, etc.), while improving the overall detection efficiency, realise remote viewing and editing of water consumption data.

2 The dimensionless expression of water quality spectral data is performed, and the obtained water quality data variables are normalised to pure quantities, and then the coincidence of normalised spectra of pharmaceutical water samples is judged. If the spectra coincide, it indicates that the parameters of the samples are similar, then they can be divided into a class; otherwise, it is divided into different categories.

3 The spectral difference between qualified samples and abnormal samples is determined by probability evaluation method. The detection object with small spectral difference between qualified samples and abnormal samples is inferior object, so as to realise the detection of pharmaceutical water quality.

2 Design of pharmaceutical water quality testing method

2.1 Multiple parameters of pharmaceutical water were collected by water quality detector

At the present stage, because there are many indicators in the water body, and the existing water quality detection methods need to test each parameter indicator in the water body in stages, there is the problem of a long detection cycle, and in this process, there is a certain probability of secondary pollution (Ruan et al., 2019). At the same time, the pharmaceutical water of inorganic hybrid nano drugs has higher requirements than ordinary water, so it is necessary to study a technology to improve the acquisition method of pharmaceutical water parameters and solve the problem of multi-parameter acquisition.

In this study, SH-3900A water quality detector was used to collect the pharmaceutical water parameters of inorganic hybrid nano drugs. The detector adopts the advanced imported optical device and structure, data with higher accuracy and stability, and can realise remote, real-time view of data, and data editing, management and comprehensive analysis, and other functions, can guarantee the inorganic hybrid nano drug pharmaceutical water parameters collected more simplicity and high efficiency (Xu et al., 2019). Figure 1 shows the SH-3900A water quality tester module.

According to Figure 1, the SH-3900A water quality detector is mainly composed of wireless module, photoelectric receiving module, photoelectric conversion module, acquisition module and control module, among which the acquisition module is the core module. The acquisition module can simultaneously collect multiple parameters, which effectively solves the limitation of traditional methods (Yotova et al., 2021). The main function of the upper computer in the process of using the detector is the control function. Under the control of the upper computer, the normal operation of each module can be realised, and contact with the main controller to ensure the safe operation of the instrument. In this detector, RS485 interface is a bright spot. With the support of this interface, the pharmaceutical water parameters and data of inorganic hybrid nano drugs

can be acquired in real time, which effectively solves the problems of long detection cycle and low detection efficiency existing in traditional methods.

Figure 1 SH-3900A water quality detector module figure

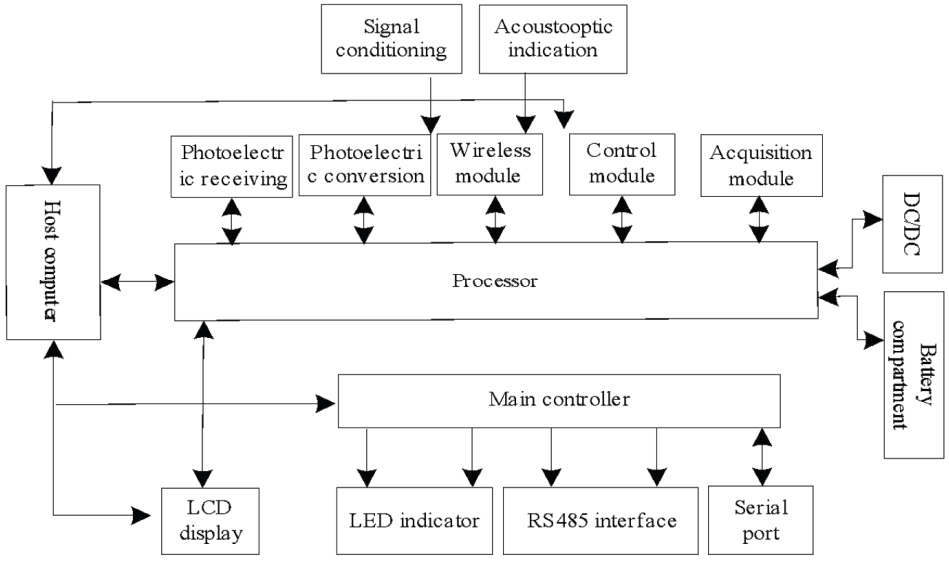


Table 1 lists the parameters of the SH-3900A water quality tester.

Table 1 SH-3900A water quality detector performance parameters

Performance parameter	*Specific value*
Wavelength range	190–1,100 nm
Optical path stability	≤ 0.002 Abs/h
Stray light	≤ 0.005%T
Spectral bandwidth	2 nm
Wavelength resolution	1 nm
Wavelength reproducibility	0.2 nm
Spectral range	200–720 nm

The water quality detector can be used to collect pH value, dissolved oxygen, microbial content, conductivity, COD, chroma, turbidity and total organic carbon at the same time.

2.2 The water samples were classified based on spectral normalisation analysis

Various parameters of pharmaceutical water were collected by SH-3900A water quality detector. Although multiple parameters can provide data basis for water quality detection, too many parameters will bring certain burden to the detection (Bownik and Wlodkowic, 2021). If these data are not divided, the accuracy of detection results will be affected and the detection workload will be increased (Dalmieda, 2019; Peng et al., 2019). Therefore, this paper classifies water sample quality based on spectral normalisation.

Normalisation refers to transforming a dimensional expression into a dimensionless expression through transformation, which aims to simplify the problem. The variables obtained by this method are scalar.

Based on the principle of spectral normalisation analysis, whether the normalised spectra of pharmaceutical water samples coincide or not is judged. If the spectra coincide, it indicates that some parameters of the samples are similar, they can be divided into a class. If the spectra do not coincide, it indicates that some parameters in the samples are inconsistent, which can be identified as obvious differences between parameters, so they need to be divided into different categories (Fang et al., 2021).

Suppose that Y represents a sample sequence, and different sample sequences together form a sample set $Y = \{y_1, y_2, \ldots, y_n\}$, where n represents the number of samples, and perform data preprocessing on the samples in this set:

$$Y^s = \frac{h^s - \mu^s}{y^s_{\max} - y^s_{\min}} \tag{1}$$

Among them, $y^s_{\max}$ and $y^s_{\min}$ respectively represent the maximum and minimum value of the sample data dimension, h^s represents the original data obtained by the collection, μ^s represents the interference item in the collected result data, and the calculation formula is:

$$\mu^s = \sum_{i=1}^{n} \sigma_i \times t_i(S) \tag{2}$$

Among them, σ_i represents the strong association between data, and $t_i(S)$ represents the closed frequent items between classes.

According to the data preprocessing results, the normalisation coefficient expression is obtained by spectral normalisation method:

$$H^2 = \frac{1}{(F/2 + F'/2)} \tag{3}$$

Among them, F represents the correlation coefficient between samples, and F' represents the lifting operator.

According to the normalisation coefficient shown in formula (3), the spectral linear coefficient can be obtained:

$$\varpi_j = H^2 \times \tag{4}$$

Among them, ω_j represents the wavelength, ∂^2 represents the average value of the spectrum, and the calculation formula is:

$$\overline{\partial}^2 = W_d x_n(k) \tag{5}$$

Among them, W_d represents the spectral reflectance, and $x_n(k)$ represents the transmission spectrum.

Since in the sample classification, there will be a variety of parameters that will affect the detection results. The sample parameters are normalised by the above-mentioned spectral normalisation method, which is represented by G_{ij}, and its expression is:

$$G_{ij} = \sum_{i=1}^{n}\sum_{j=1}^{n} dist\left(c_i, c_{ij}\right)^2 \tag{6}$$

Among them, c_i represents wavelength absorbance, and c_j represents wavelength fluctuation value. For pharmaceutical water samples, the normalisation effect is related to the wavelength fluctuation value. The degree of spectral normalisation can be measured by the specific wavelength fluctuation value (Cheng et al., 2019; Winter et al., 2019), that is, the coincidence degree of normalised spectrum, so as to realise the classification of water samples.

2.3 Detect the pharmaceutical water quality of inorganic hybrid nano drugs

The quality of classified samples will be tested. If a water pollution event occurs, it will have an immeasurable impact on drug production. Therefore, it is necessary to detect the water quality in real time in the early stage and during the pharmaceutical period, so that relevant staff can master the water use situation in time. Once a pollution event occurs, it can be handled at the first time to help reduce production losses (Zu et al., 2019).

The quality detection of pharmaceutical water for inorganic hybrid nano drugs is to detect whether various parameters and indicators in the water body meet the standards, and take preventive and response measures according to the test results (Arefin et al., 2020).

In this paper, the probability evaluation method is used to judge the spectral difference between qualified samples and abnormal samples, so as to realise the detection of pharmaceutical water quality. Firstly, the probability of possible water pollution events in the production link is calculated as follows:

$$\overline{y}_q = \frac{y_q'}{\left\|\overline{y}_q'\right\|} \Big/ M_{G_{ij}} \tag{7}$$

Among them, y_g' represents the abnormal value of sample chromaticity, $|\overline{y}_q'||$ represents the abnormal coefficient of sample, and $M_{G_{ij}}$ represents the abnormal value of sample turbidity.

And on that basis, the abnormal interval of the sample is inferred from the historical data to obtain the spectral difference between the qualified sample and the abnormal sample (Garner et al., 2021), and its expression is:

$$T = \sum_{i=1}^{n}\left(1-\xi_j\right)\times S_i \tag{8}$$

Among them, ξ_i represents the absolute difference, and S_i represents the relative difference.

The quality of pharmaceutical water for inorganic hybrid nano drugs can be effectively detected by analysing the spectral difference between qualified samples and abnormal samples.

According to the above process, on the basis of collecting multiple parameters of pharmaceutical water with water quality detector, the collection results are classified according to spectral normalised analysis results, and then the spectral difference between

qualified samples and abnormal samples is determined by probability evaluation method, so as to realise the detection of pharmaceutical water quality.

3 Experimental verification

3.1 Experimental scheme

In order to verify the effectiveness and applicability of the pharmaceutical water quality detection method for inorganic hybrid nano drugs designed in this paper, the following experimental analysis process was designed.

Taking a pharmaceutical factory as the sample collection object, 50 water samples were randomly selected from the pharmaceutical factory, and they were uniformly numbered. In the experiment, the water quality of these samples was detected, and the experimental results were processed by statistical analysis. Table 2 shows the categories of pharmaceutical water and its water quality standards.

Table 2 Pharmaceutical water categories and their water quality standards

Type	*Standard*
Drinking water	Should comply with 'Sanitary Standards for Drinking Water' (GB5749-85)
Purified water	Without any additives, the resistivity should usually be ≥ 0.5 MΩ.cm/25°C
Water for injection	Bacterial endotoxin in each 1ml water for injection should be less than 0.25 EU
Sterilised water for injection	Comply with 2000 Chinese Pharmacopoeia standard

Take the above index standards as a reference, carry out experimental analysis, and draw relevant conclusions based on the experimental results.

In order to form experimental comparison, method of Lin et al. (2019) and method of Xue (2019) were selected to compare with method of this paper, and experimental conclusions were obtained through specific numerical analysis.

3.2 Select performance indicators

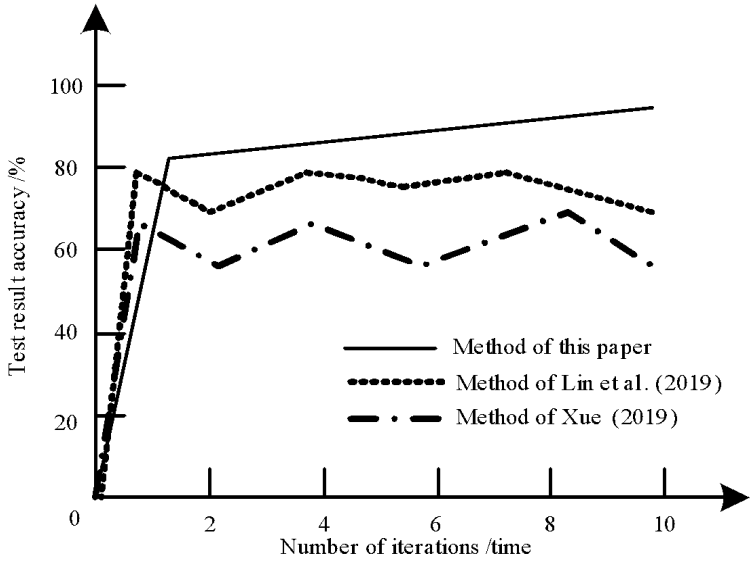
In the experiment, the application effect of the proposed method was tested by using multiple indicators, including detection result accuracy, detection time efficiency and detection process stability.

3.3 Test and analysis of performance indicators

3.3.1 Comparative analysis of accuracy of detection results

The accuracy of detection results was taken as the experimental index, and the three methods were compared. In the experiment, the number of iterations was uniformly set to 10 in order to ensure the consistency of experimental conditions. Under such conditions, the precision comparison results of detection results of different methods are shown in Figure 2.

Figure 2 The accuracy of different detection methods was compared



Analysis of the results shown in Figure 2 shows that, at the beginning of the experiment, the accuracy of water quality detection results of method of this paper is slightly lower than that of method of Lin et al. (2019) and method of Xue (2019). However, with the increase of iterations, the superiority of method of this paper becomes increasingly obvious. And the detection accuracy increased significantly. Although the growth trend of detection accuracy gradually slows down in the middle and late stage of the experiment, it is still significantly better than the traditional method.

By comparing specific experimental results and values, it can be seen that the maximum detection accuracy of method of this paper reaches about 95%, and the maximum detection accuracy of method of Lin et al. (2019) and method of Xue (2019) is about 79% and 70%, respectively. Therefore, the detection effect of method of this paper is better, which can provide help for the pharmaceutical water supervision of inorganic hybrid nano drugs and improve the quality of pharmaceutical water.

3.3.2 Comparative analysis of detection time efficiency

Taking the detection time efficiency as the experimental index, the three methods were compared, and the detection efficiency was reflected by the detection time. The shorter the detection time, the higher the detection efficiency. The detection time comparison results of different methods are shown in Table 3.

According to the data in Table 3, the minimum and maximum detection time of method of this paper are 12.5 min and 14.7 min respectively, and the minimum and maximum detection time of method of Lin et al. (2019) are 23.7 min and 26.1 min, respectively. The minimum and maximum detection time of method of Xue (2019) was 25.3 min and 31.1 min, respectively.

According to the above data, compared with the two traditional methods, method of this paper has a shorter detection time for pharmaceutical water quality, indicating its higher detection efficiency and verifying its advantages in detection efficiency.

Table 3 Statistical results of detection time by different methods / min

Number of iterations / time	*Method of this paper*	*Method of Lin et al. (2019)*	*Method of Xue (2019)*
2	12.5	23.7	25.3
4	12.8	24.5	26.0
6	13.9	25.0	26.3
8	14.5	25.6	26.7
10	14.7	26.1	31.1

3.3.3 Comparative analysis of detection process

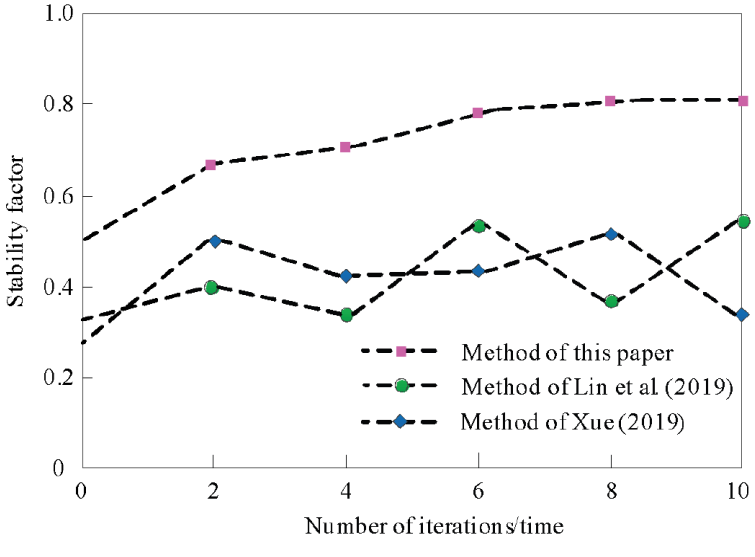
Because in the quality testing of pharmaceutical water, when there is vibration signal outside, the performance of testing equipment will change, which will affect the stability of testing results. Therefore, the stability coefficient can also reflect the effect of the detection method. Formula (9) is used to calculate the stability coefficient:

$$c(x) = \frac{\partial(x)}{D} \times \theta \tag{9}$$

Among them, $\partial(x)$ represents the intensity of the vibration signal, θ represents the fluctuation coefficient, and D represents the number of iterations.

The stability of the detection process was taken as the experimental index and the three methods were compared. The statistical results of equipment stability coefficient during the detection process by different methods are shown in Figure 3.

Figure 3 Comparison of process stability between different methods (see online version for colours)



By analysing the results shown in Figure 3, it can be seen that the stability coefficient of method of Lin et al. (2019) and method of Xue (2019) in the detection process has no obvious change trend, and the stability coefficient goes up and down. However, the stability coefficient of water quality detection process of method of this paper is higher, which is significantly higher than that of traditional methods, and keeps rising. The maximum value of the stability coefficient is close to 0.8. Therefore, the detection effect of method of this paper is more stable, which can provide reference for the safety of pharmaceutical water.

In conclusion, the inorganic hybrid nano drug pharmaceutical water quality detection method designed in this paper can detect pharmaceutical water quality at a high speed and accurately, with higher detection accuracy and stability, and can control the detection time within 15 min.

4 Conclusions

1 Considering the impact of water quality on biopharmaceutical, various detection technologies and methods emerge at the right moment, but most of the existing methods generally have problems of low accuracy of detection results, low detection efficiency and poor stability. Therefore, in order to solve the above problems, this paper proposed a pharmaceutical water quality detection method for inorganic hybrid nano drugs. On the basis of collecting related parameters of pharmaceutical water, spectral normalisation analysis was used to classify the collected results, and finally the spectral difference between qualified samples and abnormal samples was judged by probability evaluation method, so as to realise the detection of pharmaceutical water quality.

2 Experimental verification shows that the maximum detection accuracy of this method reaches about 95%, the minimum and maximum detection time are 12.5 min and 14.7 min respectively, and the maximum stability coefficient is close to 0.8. The above experimental results and data show that the detection effect of method of this paper is good and can ensure the safety of pharmaceutical water.

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