Converting *Panax ginseng* DNA and chemical fingerprints into two-dimensional barcode

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**Abstract**

**Background:** In this study, we investigated how to convert the *Panax ginseng* DNA sequence code and chemical fingerprints into a two-dimensional code. In order to improve the compression efficiency, GATC2Bytes and digital merger compression algorithms are proposed.

**Methods:** HPLC chemical fingerprint data of 10 groups of *P. ginseng* from Northeast China and the internal transcribed spacer 2 (ITS2) sequence code as the DNA sequence code were ready for conversion. In order to convert such data into a two-dimensional code, the following six steps were performed: First, the chemical fingerprint characteristic data sets were obtained through the inflection filtering algorithm. Second, precompression processing of such data sets is undertaken. Third, precompression processing was undertaken with the *P. ginseng* DNA (ITS2) sequence codes. Fourth, the precompressed chemical fingerprint data and the DNA (ITS2) sequence code were combined in accordance with the set data format. Such combined data can be compressed by Zlib, an open source data compression algorithm. Finally, the compressed data generated a two-dimensional code called a quick response code (QR code).

**Results:** Through the abovementioned converting process, it can be found that the number of bytes needed for storing *P. ginseng* chemical fingerprints and its DNA (ITS2) sequence code can be greatly reduced. After GTC2Bytes algorithm processing, the ITS2 compression rate reaches 75% and the chemical fingerprint compression rate exceeds 99.65% via filtration and digital merger compression algorithm processing. Therefore, the overall compression ratio even exceeds 99.36%. The capacity of the formed QR code is around 0.5k, which can easily and successfully be read and identified by any smartphone.

**Conclusion:** *P. ginseng* chemical fingerprints and its DNA (ITS2) sequence code can form a QR code after data processing, and therefore the QR code can be a perfect carrier of the authenticity and quality of *P. ginseng* information. This study provides a theoretical basis for the development of a quality traceability system of traditional Chinese medicine based on a two-dimensional code.

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1. Introduction

*Panax ginseng* is a worldwide popular herbal medicine, which has been used in traditional Asian medicine for thousands of years. Since the quality of *P. ginseng* depends on many conditions and factors, the most fundamental problem to be solved is the authenticity and evaluation model of quality level issue, which involves a lot of information. Therefore, it is essential to design a very simple and easy information carrier to carry the related quality information. The current use of DNA sequences to identify true and false methods has been widely recognized [1,2]. Meanwhile, chemical fingerprints form the industry’s widely accepted evaluation model of quality level [3–7]. If these two kinds of *P. ginseng* information can be represented by the current popular two-dimensional code information carrier, the final consumer can easily trace the quality of *P. ginseng* using a smartphone, which will
promote the development and application of a P. ginseng quality traceability system.

More convenient traditional Chinese medicine quality information carrier has been studied. Chen et al [8] found that the internal transcribed spacer 2 (ITS2) sequence code is more appropriate for identifying medicinal plant species. Liu et al [9] studied the conversion of the Chinese herbal medicine DNA sequence into a quick response code (QR code). Kumar et al [10] studied the conversion of DNA barcoding into PDF417. Cai et al [11] studied the conversion of Chinese medicine chemical fingerprints into a QR code. However, the two-dimensional code storage space is very limited; the original data of the normal P. ginseng DNA sequence and chemical fingerprints far exceed the capacity of the current two-dimensional codes. Therefore, compression algorithms for P. ginseng DNA sequence and chemical fingerprint data are very important. Many methods are used for compression of DNA sequences; some effective methods are BioCompress-2 [12], GenCompress [13], CTW + LZ [14], DNA Compress [15], DNAPack [16], DNADP [17], GeNML [18], and so on. Currently, the main processing step for chemical fingerprints is to find the inflection point in the filtering process [11]. The subsequent compression algorithm is to be studied in the future.

Based on the existing studies of conversion of traditional Chinese medicine chemical fingerprints into two-dimensional codes [11], in this study, we explored a novel way to further convert the P. ginseng DNA (ITS2) sequence code and chemical fingerprints into a QR code to record authenticity information and quality information of ginseng.

2. Materials and methods

2.1. Materials

This study was carried out on HPLC chemical fingerprint data of 10 groups (Agilent rapid detection method) of roots and fibrous roots of ginseng from Northeast China, grown for 2–6 years. The ITS2 sequence code was selected as the DNA sequence code for its species. Moreover, HPLC chemical fingerprint data of P. ginseng were obtained from the State Key Laboratory of Quality Research in Chinese Medicine, University of Macau. The ITS2 sequence code data were acquired from the Chinese pharmacopoeia medicine DNA barcoding standard sequence [8,19]. Meanwhile, Cai et al [11] found the QR code very suitable for carrying chemical fingerprints of traditional Chinese medicine by comparing the popular two-dimensional code QR code, data matrix, PDF 417, and other formats. In this study, since we only need add DNA (ITS2) sequence code on the basis of the original, there is no need to choose any other two-dimensional code. Therefore, the QR code was suitable for use as our target two-dimensional code.

In this study, data processing was completed with Ruby language (v1.9.3 p551), the Excel spreadsheet was operated by a third-party plug-in named Gem spreadsheet 0.9.8, and the QR code was created by a third-party plug-in named Gem qrrcode 0.7.0. The program could run on the operating system of Windows XP/Windows 7/Windows 8. Fig. 1 shows a flowchart of whole conversion processes.

2.2. Six steps of two-dimensional code conversion

2.2.1. Step 1: Obtaining chemical fingerprint data set of key feature points

The original data of P. ginseng chemical fingerprints were obtained from Agilent equipment output file, and the original contents of the file are shown in Fig. 2 (test results of the fibrous roots of a 4-year-old ginseng).

The key data set (time—value) of chemical fingerprints in the output file was saved in an Excel file format due to the text-formatted output file. “Time” represents duration of detection in minutes, while “value” represents detected absorption values in that minute. The number of data points was about 5,000 or so (about 104K bytes), which is beyond the capacity of the current variety of any two-dimensional code format. Thus, the data needed to be filtered before being converted into a two-dimensional code. According to the selected inflection point filtering algorithm [11], we needed to collect the data of the key feature points (inflection points) of P. ginseng chemical fingerprints. Inflection point features are shown in Fig. 3 and inflection point judgment conditions in Fig. 4. “Time” represents the detection duration in minutes and “value” represents the absorbance value corresponding to the detected time.

Compared with the filtering algorithm proposed earlier [11], this study proposed mainly the following two improvements:

(1) Time accuracy was up to two decimal places, while time accuracy had been up to one decimal place in the original paper.
Fig. 2. Part of the original data from 4-year-old P. ginseng fibrous root test results (Agilent rapid detection method).

Table 1 lists the data results after implementing the filtering algorithm.

2.2.2. Step 2: Digital merger compression based on digital data sets of chemical fingerprinting

Digital merger compression (DMC) was proposed due to the digital feature of chemical fingerprints. Time data and mAu data were amplified 100 times and 10 times, respectively, in order to obtain integers. Then the data could be combined into an array of 2 bytes, 3 bytes, or 4 bytes according to its size. More details of the algorithm are shown in Fig. 5.

Using the DMC algorithm, data sets of chemical fingerprinting completed the precompression processing. Table 2 lists the data changes after running the DMC algorithm.

2.2.3. Step 3: Conversion of ginseng DNA (ITS2) sequences code into bytes (GTCA2 bytes)

The P. ginseng DNA (ITS2) sequence code was 230 bytes when we chose 70 characters per line breaks, as shown in Fig. 6.

Each of the four bases (G, T, C, and A) was represented by 2 bits (00, 01, 10, and 11, respectively) according to the features of P. ginseng DNA (ITS2) sequence code. The first two bytes were used to save the total length of the sequence code within 65,535 base sequence. Therefore, it became a byte algorithm (GTCA2Bytes) by transition, as shown in Fig. 7.

2.2.4. Step 4: Chemical fingerprint data and DNA (ITS2) sequence code data combined by a predefined data format

To ensure that the converted two-dimensional code of traditional Chinese medicine chemical fingerprints can be identified and reproduced, the compressed array of bytes needs to be combined in accordance with the set data format. The available common standard formats are XML, JSON, etc. However, it requires additional bytes, which is not proper for the two-dimensional code due to its limited data capacity. Therefore, a combination of simpler rules was adopted in this study.

The compressed byte array of DNA (ITS2) sequence and byte array of chemical footprints were combined with the following format, in which “||” was chosen to separate arrays, as shown as follows:

2 bytes array of ITS2 sequence || 2 bytes array of chemical fingerprint data || 3 bytes array of chemical fingerprint data || 4 bytes array of chemical fingerprint data

2.2.5. Step 5: Compression of combined data by Zlib

The combined data needed to be compressed in advance in order to get less data. Many algorithms of compression are available, which are divided into two major categories of lossy and lossless compression. Owing to nondestructive reduction, the most common Zlib (DEFLATE RFC 1951, variation of the LZ77 algorithm [20,21]) lossless compression algorithm was suitable for this study.
The chemical follows. The results of the four processes are analyzed as data; in this study, four processes were used to reduce the number transformed into a QR code. A very important purpose of the compression algorithm has the advantage of high efficiency compared with other compression algorithms, this compression was adopted due to the small DNA sequence code of P. ginseng DNA (ITS2) sequence code. Through the algorithm, the number of bytes could be reduced to nearly 75%.

The fourth process involved the Zlib compression algorithm, corresponding to Step 5. Table 3 shows the changes in the number of bytes after the implementation of the Zlib compression algorithm. Compared with the number of data bytes before compression, the compression ratio was between 87.2% and 94.85%, while compared with the original data, the compression rate was between 0.48% and 0.64%. After the six-step process, the P. ginseng DNA (ITS2) sequence code and chemical fingerprints were successfully converted into a QR code. The results of the operation are shown in Figs. 8 and 9 for the selected four groups of data.

By converting the 10 groups of data into a QR code, we could find that the number of bytes for ginseng chemical fingerprints and DNA (ITS2) sequence code was significantly reduced after treatment. The DNA (ITS2) sequence code compression rate could reach 75%. After filtering the chemical fingerprints and DMC algorithm processing, the compression rate could be more than 99.65%. Finally, the overall compression ratio was over 99.36%, and the capacity of the QR code was about 0.5 kilobytes (KB).

### 4. Discussion

In this study, on the basis of the conversion of the DNA (ITS2) sequence code [9,10] as well as the chemical fingerprints into a two-dimensional code [11], further research was carried out. The P. ginseng DNA (ITS2) sequence code and HPLC chemical fingerprinting were converted into a two-dimensional code in accordance with certain procedures and formats. GATC2Bytes and DMC algorithms were used in this conversion process. After compression by Zlib, QR code bytes were about 0.5 KB, which is far less than converting chemical fingerprint QR code method proposed by Cai et al [11]. Using their method, the number of bytes in the two-dimensional code was found to be between 1 KB and 2 KB. Compared the QR code conversion method with theirs, DMC and Zlib compression processing made the number of bytes of QR code less nearly between 50% and 75%.

Many DNA sequences compression algorithm are available [12–18]; most of them have been proposed to solve the issue of DNA sequence, which is very large—more than 100 million petabytes [22]. In this study, the simple GATC2Bytes compression algorithm was adopted due to the small DNA sequence code of P. ginseng, which is less than 1 kb. After processing, the number of bytes can be reduced by 75%, which can be improved further. We promote a novel method to compress the chemical fingerprint code by the DMC algorithm. Since no similar literature reports are available, further research is required.

Furthermore, the converted two-dimensional code can be recognized by a computer and be restored to the original DNA (ITS2) sequence and chemical fingerprint data, the process of which has been proved to be reversible.

Traditional Chinese medicine chemistry (composition) fingerprinting methods are mainly based on spectroscopy and
chromatography: UV, IR, MS, NMR, TLC, GC, HPLC, capillary electrophoresis, and so on. Among them, HPLC has become the primary means of fingerprint research currently. This study focuses on the conversion of HPLC and DNA (ITS2) sequence, due to its chemical fingerprint data form and DNA (ITS2) sequence have many similarities, so six steps conversion method should be applicable to some of the traditional Chinese medicine.

During the experiment, we found that how to compress the space was an important challenge. DNA (ITS2) may be replaced by other ways (for example, SNP) to reduce space. In addition, recording only the major chemical fingerprints is a very good idea for space compression. However, it will cause problems with incomplete information [23,24]. Therefore, we finally chose to use DNA (ITS2) and complete chemical fingerprints for this experiment.

Time complexity should be considered within this experiment. If the time complexity cannot be reduced, the experiment does not have practical significance. As shown in Table 4, 10 sets of data conversion processes were tested (Computer Environment: Sony VAIO with window XP sp3, 3G memory, dual-core, Intel CPU: 1.8GHz). We found that the average total time for the conversion of 10 sets of data was 11.675 s, which was within the acceptable range.
Conversion of P. ginseng DNA (ITS2) sequence and chemical fingerprints into a two-dimensional code can be explored further. While a QR code can carry a maximum of 2,953 bytes, our experiment used only about 500 bytes, leaving a large amount of space to carry more related information. If the P. ginseng DNA (ITS2) sequence and chemical fingerprints can be converted into a two-dimensional code successfully and easily, then it will be simple and convenient for a customer to trace the P. ginseng quality by a smartphone. Therefore, this method is a solid foundation of a P. ginseng quality traceability system.

4.1. Limitation and future research

This paper presents only the conversion of the P. ginseng DNA (ITS2) sequence and the HPLC chemical fingerprint data of 10 groups detected by Ailent Quick test into a two-dimensional code. Whether the DNA and chemical fingerprints of other medicines detected by other instruments can be smoothly converted into a two-dimensional code requires further research.

By analyzing the above discovery process, P. ginseng fingerprints and Chinese medicine DNA (ITS2) sequences must be filtered and must undergo compression processing before being converted into a two-dimensional code. In the present study, there should be room for optimization in the second-step HPLC chemical fingerprint compression (DMC) algorithm and third-step DNA (ITS2) sequence compression algorithm (GTCA2Bytes). Furthermore, the fourth-step selection of the data format combinations "||" for separation, there need to be perfected.

5. Conclusions

This study presents six steps to convert the P. ginseng DNA (ITS2) sequence code and chemical fingerprints into a QR code. In order to improve the compression ratio, this study proposes a simple GATC2Bytes compression algorithm for the compression of DNA (ITS2) sequence code and a DMC preprocessing algorithm for early treatment of chemical fingerprints. This study shows that the P. ginseng DNA (ITS2) and the chemical fingerprint information can be stored in a two-dimensional code. This study provides a theoretical basis for building a P. ginseng quality tracing system based on the two-dimensional code that contains quality information.
The authors declare that they have no competing interests.

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References

[1] Luo K, Chen S, Chen K, Song J, Yao H, Ma X, Zhu Y, Pang X, Yu H, Li X, et al. Assessment of candidate plant DNA barcodes using the Rutaceae family. Sci China Life Sci 2010;53:701–8.

[2] Selvaraj D, Sarma RK, Shanmughanandhan D, Srinivasan R, Ramalingam S. Evaluation of DNA barcode candidates for the discrimination of the large plant family Apocynaceae. Plant Syst Evol 2015;301:1263–73.

[3] Yan SK, Xin WF, Luo GA, Wang YM, Cheng YY. An approach to develop two-dimensional fingerprint for the quality control of Qingkailing injection by high-performance liquid chromatography with diode array detection. J Chromatogr A 2005;1090:90–7.

[4] Xie YY, Luo D, Cheng YJ, Ma JF, Wang YM, Liang QL, Luo GA. Steaming-induced chemical transformations and holistic quality assessment of red ginseng derived from Panax ginseng by means of HPLC–MS/MS n-based multi-component quantification fingerprint. J Agric Food Chem 2012;60:8213–24.

[5] Lu GH, Chan K, Liang YZ, Leung K, Chan CL, Jiang ZH, Zhao ZZ. Development of high-performance liquid chromatographic fingerprints for distinguishing Chinese Angelica from related umbelliferae herbs. J Chromatogr A 2005;1073:383–92.

[6] Liu L, Wang Y, Song Q, Bao YP. Fingerprint identification system based on two-dimensional barcode and DSP. Adv Mater Res 2012;479:2082–3.

[7] Chen SL, Yao H, Han JP, Liu C, Song YJ, Shi LC, Zhu YJ, Ma XY, Gao T, Pang XH, et al. Validation of the ITS2 region as a novel DNA barcode for identifying medicinal plant species. PLoS One 2010;5:e8613.

[8] Korodi G, Tabus I. Normalized maximum likelihood model of order-1 for the compression of DNA sequences. In: Data Compression Conference, 2007. DCC’07. IEEE; 2007. p. 33–42.

[9] Kreft S, Navarro G. Self-indexing based on LZ77. CPM 2011;11:41–54.

[10] Kumar NP, Rajavel A, Jambulingam P. Application of PDF417 symbology for ‘DNA barcoding’. Comput Meth Prog Biomed 2008;90:187–9.

[11] Cai Y, Li XW, Li M, Chen XJ, Hu H, Ni JY, Wang YT. Traceability and quality control in traditional Chinese medicine: from chemical fingerprint to two-dimensional barcode. Evid Based Complement Altern Med 2015, 251304. http://dx.doi.org/10.1155/2015/251304. 6 pages.

[12] Grumbach S, Tahi F. A new challenge for compression algorithms: genetic sequences. Inform Process Manag 1994;30:875–86.

[13] Chen X, Kwong S, Li M. A compression algorithm for DNA sequences. IEEE Eng Med Biol 2010;20:61–6.

[14] Matsumoto T, Sadakane K, Imai H. Biological sequence compression algorithms. Genome Inform 2000;11:43–52.

[15] Chen X, Li M, Ma B, Tromp J. DNA Compress: fast and effective DNA sequence compression. Bioinformatics 2002;18:1696–8.

[16] Behzadi B, Le Fessant F. DNA compression challenge revisited: a dynamic programming approach. Comb Pattern Match 2005;3537:190–200.

[17] Srinivasa KC, Jagadish M, Venugopal KR, Patnaik LM. Efficient compression of non-repetitive DNA sequences using dynamic programming. In: Advanced Computing and Communications, ADCOM 2006, International Conference on IEEE; 2006. p. 569–74.

[18] Deutsch P, Gailly J. Zlib compressed data format specification version 3.3 (No. RFC 1950). RFC 1950, May.

[19] Galperin MY, Cochrane GR. Petabyte-scale innovations at the European nucleotide archive. Nucl Acids Res 2009;37:D1–4.

[20] Xie PS, Leung AY. Understanding the traditional aspect of Chinese medicine in order to achieve meaningful quality control of Chinese materia medica. J Chromatogr A 2009;1216:1933–40.

[21] Liang Y, Xie P, Chan K. Perspective of chemical fingerprinting of Chinese herbs. Planta Med 2010;76:1997–2003.