Application of Library Search Techniques of FTIR Fingerprint for
the Identification of Traditional Chinese Herbal Medicine

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in
Chemistry

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My sincere thanks also go to Mr. Tsai Sam Hip and Miss Lee Tin Wan for their valuable advice, suggestion and technical support during the course of research. I would also thank my family and my friends for their support and help.

Finally, I would like to thank Jesus for his Love and hope the world will be peaceful.

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Abstract

Identification of all Chinese herbal flowers collected in Pharmacopoeia of the People's Republic of China was achieved by Library Search Techniques using Fourier Transform Infrared Spectroscopy (FTIR). Euclidean search method and Soft Independent modeling of Class Analogy (SIMCA) classification method were used as library search techniques to identify herbal samples by comparing infrared spectra database of extracts. A Chinese-herbal-flower library search database composed of twenty-one species was built up in each method. The IR spectrum shows the characteristic of a mixture rather than that of a pure compound.

The Euclidean search method compares the shape of the sample spectrum with that of known spectra in a Chinese-herbal-flower library, producing an Euclidean Hit List, which is a list of extracts whose spectra most closely match that of the sample.

In the SIMCA classification method individual class models for each Herb were built and calibrated using the QUANT+ software. SIMCA diagnostics and validation tests were performed to check the validity of the model before classifying unknown flower extracts.

In this study, it was found that both Euclidean search method and SIMCA classification method are suited for the IR spectra identification; however, the SIMCA classification method gives a better recognizing and rejection abilities for the unknown samples respective when compared with the library standards, but the Euclidean search method is quicker and more convenient for use.
Abbreviations

IR     Infrared Spectroscopy
EM     Electromagnetic
FTIR   Fourier Transform Infrared Spectrometer / Spectrometry
TCM    Traditional Chinese Medicine
QC     Quality Control
SDA    State Drug Administration
FDA    Food and Drug Administration
SIMCA  Soft Independent Modeling of Class Analogy
RSD    Relative Standard Deviation
本論文研究了運用傅里葉紅外分光光譜法分辨在中華人民共和國藥典上所收集的一些花類中藥。

論文利用了統一的提取方法，對 21 種花類中藥標準品進行了提取，並建立了提取物紅外光譜庫。然後利用歐氏 (Euclidean) 以及 SIMCA 紅外光譜檢索技術對該 21 種中藥的樣品的光譜圖進行分辨。

實驗結果顯示兩種方法均能正確分辨出藥材樣品，其中 SIMCA 方法的分辨能力上比歐氏方法較強，而 Euclidean 方法較快捷方便。
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Chapter 1

Introduction

1.1 Basic theory of FTIR

1.1.1 Infrared Spectroscopy

Infrared (IR) radiation refers to the part of the electromagnetic spectrum between the visible and microwave regions, involving the class of electromagnetic (EM) radiation with frequencies between 4000 and 400 wavenumbers (cm\(^{-1}\)).

The IR spectroscopy involves collecting absorption information and analyzing it in the form of a spectrum. The resulting spectrum represents the molecular absorption and transmission, creating a molecular fingerprint of the material, which corresponds to the frequencies of vibrations between the bonds of the atoms making up the material. Chemical bonds in different environments will absorb varying intensities and at varying frequencies. Because each compound is a unique combination of atoms, no two compounds produce exactly the same infrared spectrum. Therefore, infrared spectroscopy can result in a positive identification of different kinds of material.\(^1\) The size of the peaks in the spectrum is a direct indication of the amount of material present.
Infrared spectroscopy can also be used in the analysis of mixture. The resulting spectrum of a mixture is the sum of the absorption and transmission of all compounds in the mixture, producing a characteristic fingerprint spectrum of the mixture. Although the interpretation of functional group of a mixture spectrum was very difficult, by comparing unknown spectrum with reference spectra, the unknown mixture can be identified and the quality or consistency of a sample can be determined.\textsuperscript{2-4}

\subsection{Dispersive Infrared Spectrometer}

The original infrared instruments were of the dispersive type. These instruments separated the individual frequencies of energy emitted from the infrared source by the use of a prism or grating. The detector measures the amount of energy at each frequency which has transmitted through the sample. This results in a spectrum, which is a plot of intensity against frequency.
1.1.3 Fourier Transform Infrared Spectrometer (FTIR)

FTIR stands for Fourier Transform Infrared, the preferred method of infrared spectroscopy. FTIR spectrometry was developed in order to overcome the limitations encountered with dispersive instruments, which has a main difficulty of slow scanning process.

It collects an interferogram of a sample signal using an interferometer and then performs a Fourier Transform on the interferogram to obtain the spectrum.
Figure 1.2 shows the schematic of the interferometer. The interferometer takes a beam of light, and splits it into two beams by a beam splitter. When the distance of the movable mirror from the beam splitter changes, it makes one of the light beams travel a different distance than the other. The difference in distance travelled by these two light beams is called the optical path difference. After the two beams combined together, different wavelengths of radiation are in-phase and out-of-phase at a frequency that is dependent both upon the rate at which the mirror moves and the frequency of radiation. The complex pattern of overlaid sinusoidal waves of light is known as an interferogram. The interferogram can be converted back to the original frequency distribution by means of a Fourier transform by computer.
1.1.4 Advantages of FTIR

1.1.4.1 Multiplex advantage

In an FTIR spectrometer all wavelengths are collected simultaneously whereas in dispersive type wavenumbers are observed sequentially as grating is scanned. When spectra are collected under identical conditions on dispersive and FTIR spectrometers, the signal-to-noise ratio of the FTIR spectrum will be greater than that of dispersive spectrum by a factor of \( N^{1/2} \) where \( N^{1/2} \) is the number of resolution elements.\(^1\)

1.1.4.2 Throughput advantage

All the infrared radiation passes through the sample and strikes the detector at once in an FTIR spectrometer. There is no slit to restrict the wavenumber range and reduce the intensity of infrared radiation that strikes the detector. Therefore, the detector sees the maximum amount of light at all points during a scan.

An instrument with a high signal to noise ratio will be more sensitive, be applicable to weak signals and more kinds of samples, and allow absorbance to be measured more accurately than an instrument with a low signal to noise ratio.
1.2 Traditional Chinese Medicine (TCM)

Traditional Chinese medicine has existed for thousand years. It appeared in ancient China as far as in the Shen Nong Pen T’sao Jing (神農本草經) or Emperor Shen Nong’s Classic Herbal, which was published in 200 BC and believed to be the earliest medical monograph of China. There is no doubt that TCM is useful for treating many kinds of illness. The main function of TCM is treating the acute diseases and conditions such as killing bacteria or a virus; healing chronic illness such as gastrointestinal disorder, respiratory disorder, allergies, immune system deficiency by strengthening the body, helping it to recover and maintaining daily life health by keeping the balance of human body.

In recent years, TCM is getting more attention. Because of the realization of limitation of western approach, people are seeking alternative approach to boost up the body against ageing, cancer, AIDS, and various immune diseases. TCM is suitable for these sorts of disease by aiming to stimulate the body's support mechanism to enable it to heal itself. Moreover the combination of western approach and the TCM approach in treating diseases become more and more popular. Many people believe that it is more efficient and useful. TCM is also gaining global popularity as alternative medicine and health supplements and expands rapidly in
most western countries.

However, the efficiency of TCM can be highly affected by the quality of the raw material while the quality of the raw material and product may vary dramatically due to different species, location, growth season, maturation and so on.\textsuperscript{6}

There are some causes for the large quality variation of TCM. Firstly, the description of the shape and appearance of the TCM in the Chinese material Medica is too simple. Secondly, there are plenty of alternative given name(s) and place of origin of a TCM, which makes people feel ambiguous and difficult to classify the medicine. Thirdly, due to the different custom and dialect between different places in China, different TCM may have similar or even have the same name and are being mixed up. Fourthly, some TCM may have similar appearance and mis-recognized and collected wrongly. Fifthly, when the supply of one TCM is unable to meet the demand, some merchants may use another TCM as substitute. Sixthly, some tradesmen play tricks or mix the spurious one with the genuine one in order to earn more money. The more expensive the TCM is, the more the fake product exists in the market.
Therefore, there are fake or poor quality herbal drugs in the market. These substances may be ineffective and even lethal.\textsuperscript{7-8} One of the key factors in prompting the TCM based products in international market is to have good quality control (QC). For this reason, the identification of Chinese herbal drugs is very important. The Chinese government is highly supportive of this modernization of TCM.\textsuperscript{9}

1.3 Identification of Traditional Chinese Herbal Medicine

1.3.1 Traditional method for the Identification of TCM

The identification of traditional Chinese medicine has a long history. It started from Shen Nong Pen T’sao Jing (神農本草經), which collected 365 medicines from plants, animals and minerals with a description and function of the medicines. Before the 19\textsuperscript{th} century people used experience to identify medicine. After that four main identification methods, namely, source identification, trait identification, microscopic identification and physicochemical identification, gradually become widely used for the identification of TCM.\textsuperscript{10}
1.3.2 Instrumental method for the Identification of TCM

Nowadays, in order to get more accurate and reliable identification, modern identification methods, mainly instrumental analysis methods, have been developed and applied. It includes chromatography, spectroscopic methods, molecular biological technique, electrophoresis, artificial neural networks, fingerprint method and so on.\textsuperscript{10-16}

1.3.2.1 Identification of TCM using fingerprint method

Usually, certain active ingredients of the TCM are being analyzed quantitatively to guarantee the quality of the Medicine. However, Chinese medicine is very complex and intricate.\textsuperscript{4} The integration of the ingredient components of whole medicine is very important towards its function. Therefore, it will be the trend that the analytical chemistry develops from microanalysis towards macro analysis of the whole medicine.\textsuperscript{17} TCM now requires some comprehensive evaluation measure to assess the quality of the Chinese herbal medication.

Fingerprint is one of the feasible approaches to be a more comprehensive and more effective for the quality assessment of Chinese herbal medication.\textsuperscript{18-20}
Since different kinds of medicine have different components and composition of compounds, each kind of medicine would have its own fingerprint infrared spectrum. Hence it can be used for the identification of TCM. Fingerprint infrared spectroscopy plays an important role in the quality control and identification in chemical and pharmaceutical industries. A lot of efforts are now put on the research and development of fingerprinting of TCM. It is preferred and supported by the State Drug Administration (SDA) and accepted by Food and Drug Administration (FDA).

Some researchers identified Chinese herbal drugs just by visual comparison of the intensity and wavenumber of the peaks of the spectral fingerprints. In order to be more accurate and to reduce the time consumed, spectral fingerprints should be quantified and the comparison should be handled by computers.

### 1.3.3 Identification of TCM using FTIR fingerprint method

An FTIR fingerprint of a TCM represents the integration of IR spectra of the whole content of the TCM. Since every TCM has a unique chemical content, some researchers have used FTIR fingerprinting method to identify TCM. Moreover, different TCM can be analysed by using the same solvent system rather than
changing the solvent system for every TCM. Therefore this method is suitable for building up fingerprint library database.

1.4 Objective

The objective of this research is to apply FTIR fingerprinting method to identify the traditional Chinese herbal flowers collected in *Pharmacopoeia of the People’s Republic of China*. A database of these herbs was built. Two Library search techniques, namely, Euclidean and SIMCA were applied to identify the TCM.
In this research, all the procedures were standardized. Samples were collected followed by extraction of ingredients. IR analysis and data processing were then performed. Part of the data was stored to a Library database and part of the data was treated as sample to be identified using the library database. Figure 2.1 shown the outline of the method.
2.2 Reagents and glassware

Analytical grade dichloromethane from Lab-Scan and Fisher Chemical was used for extraction. Deionized water was used for extraction and washing. Analytical grade 95% calcium chloride from Aldrich was used in the drying process. Spectroscopy grade potassium bromide purchased from Merck was used to prepare the KBr pellets. All glassware was washed thoroughly with detergent and rinsed with deionized water and dried with an oven.

2.3 Instrumentation

Perkin Elmer model 1615 FTIR spectrometer with a lithium tantalite standard detector was used to measure the IR spectra. A Corning hot plate stirrer was used for decoction. A Wig-L-Bug amalgamator model 3110b was used to mix the sample extract with KBr and grind the mixture to fine powder. An Aldrich macro-micro KBr pellet die was used to prepare the KBr pellets for the IR analysis.

2.4 Library search program

Soft Independent Modeling of Class Analogy (SIMCA), which is a commercial-available software program produced by Perkin-Elmer Limited was employed.
Euclidean Search is in a software package of spectrum 3.01 also produced by Perkin-Elmer Limited was also employed for the research.

2.5 Samples

Twenty-one species of Chinese Herbal flowers are collected in Pharmacopoeia of People's Republic of China, which is a national code of standards for the quality of drugs. In this research, 64 samples in total from the twenty-one species were used. They were collected from Hong Kong retail shops, the School of Chinese Medicine of the Chinese University of Hong Kong and National Institute for the Control of Pharmaceutical and Biological Products.

The Chinese name, Latin medicine name and the number of sample of each species of herbal flowers are listed in Table 2.1. The listed symbols will be used to represent the corresponding flowers in the subsequent part of this thesis.
<table>
<thead>
<tr>
<th>Symbol used</th>
<th>Chinese Name</th>
<th>Latin Medicine Name</th>
<th>Chinese Name Spelling</th>
<th>No. of sample collected</th>
</tr>
</thead>
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<td>hhh</td>
<td>合歡花</td>
<td>Flos albizia</td>
<td>Hehuanhua</td>
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</tr>
<tr>
<td>mm</td>
<td>密蒙花</td>
<td>Flos buddlejae</td>
<td>Mimenghua</td>
<td>3</td>
</tr>
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<td>凌霄花</td>
<td>Flos campsis</td>
<td>Lingxiaohua</td>
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<td>紅花</td>
<td>Flos carthami</td>
<td>Honghua</td>
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<td>丁香</td>
<td>Flos caryophylli</td>
<td>Dingxiang</td>
<td>4</td>
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<tr>
<td>jgh</td>
<td>雞冠花</td>
<td>Flos celosiae cristate</td>
<td>Jiguanhua</td>
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</tr>
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<td>菊花</td>
<td>Flos chrysanthemi</td>
<td>Juhua</td>
<td>4</td>
</tr>
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<td>Yejuehua</td>
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<td>Flos daturae</td>
<td>Yangjinhua</td>
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<td>Flos ericauli</td>
<td>Guijingcao</td>
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<td>kdh</td>
<td>款冬花</td>
<td>Flos fararae</td>
<td>Kuandonghua</td>
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<td>yh</td>
<td>芸花</td>
<td>Flos genkwa</td>
<td>Yuanhua</td>
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<tr>
<td>jyh</td>
<td>金銀花</td>
<td>Flos loicerae</td>
<td>Jinyinhua</td>
<td>4</td>
</tr>
<tr>
<td>sfh</td>
<td>旋覆花</td>
<td>Flos inulae</td>
<td>Xuanfuhua</td>
<td>2</td>
</tr>
<tr>
<td>xy</td>
<td>辛夷</td>
<td>Flos magnoliæ</td>
<td>Xinyi</td>
<td>4</td>
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<td>hph</td>
<td>厚朴花</td>
<td>Flos magnoliæ officinalis</td>
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<td>Flos mume</td>
<td>Meihua</td>
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<td>ygh</td>
<td>月季花</td>
<td>Flos rosae chinensis</td>
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<td>Flos rosae rugosae</td>
<td>Meiguihua</td>
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</tr>
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<td>hh</td>
<td>槐花</td>
<td>Flos sophorae</td>
<td>Huaihua</td>
<td>5</td>
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</tbody>
</table>
2.6 Sample pretreatment

Samples were identified by Professor Hu Shiu Ying, Honorary Professor of Chinese Medicine, and were then stored in a clean dry plastic bag ready for use.

2.7 Extraction of ingredients

In the extraction part, about 5g of each sample was put into a 250-ml beaker and was boiled with 150 ml of deionized water to 50 ml by a heater. The mixture was filtered by suction filtration and washed with 20 ml of deionized water. The filtrate was transferred to a 100-ml separating funnel and extracted with 20 ml of dichloromethane four times. The organic layers were collected in a 100-ml conical flask, dried with anhydrous calcium chloride and then filtered by a filter funnel to a 100-ml conical flask. The filtrate was evaporated to about 2 ml by a rotary evaporator, and then transferred to a 5-ml vial containing about 0.2g of KBr. It was evaporated by a rotary evaporator until dried. The KBr mixture was used to prepare KBr pellet for collecting the IR spectrum.
2.8 Preparation of KBr pellet

About 0.1g of the dried KBr mixture was mixed with about 0.3g of KBr powder and a Plexiglas ball pestle in a 1-ml stainless steel sample holder. It was shaken with a Wig-L-Bug amalgamator for 30 seconds for three times in a 10 seconds interval. Then the Plexiglas ball pestle was removed from the sample holder. The KBr mixture in the sample holder was ground again with the Wig-L-Bug amalgamator for 30 seconds twice in a 10 seconds interval. About 200mg of the ground KBr mixture was transferred to a KBr pellet die which was then pumped for 3 minutes to remove the gaseous and water vapor trapped in the KBr mixture. Then, the die was pumped for another 2 minutes with 8 tons of pressure on the die. After that the KBr pellet disc was obtained and was held by a sample holder and put in the FTIR spectrometer to collect the spectrum of the sample. The time of exposure for the KBr mixture and pellet should be kept as short as possible to prevent the reaction of KBr and water.

2.9 IR spectrum measurement

The IR spectrum was collected in absorbance for the spectral range 4000cm\(^{-1}\) – 400cm\(^{-1}\) with sampling interval of 2cm\(^{-1}\) with resolution: 8cm\(^{-1}\) with 64 scans. The data range was 2000cm\(^{-1}\) – 700cm\(^{-1}\).
2.10 Data processing

The spectrum was smoothed at 5 points using block average algorithm and normalized to 1.42.

2.11 IR Database

The spectra of the twenty-one flowers extract were collected and used for building the IR library database. These spectra are shown from Figure 2.2 to figure 2.22.

Figure 2.2 Flos caryophylli (丁香)
Figure 2.3 *Flos ericauli* (谷精花)

Figure 2.4 *Flos carthami* (紅花)
Figure 2.5 *Flos Sophorae* (槐花)

Figure 2.6 *Flos Albizia* (合歡花)
Chapter 2: Experimental

Figure 2.7 *Flos magnoliae officinalis* (厚朴花)

Figure 2.8 *Flos celosiae cristate* (雞冠花)
Chapter 2: Experimental

Figure 2.9 *Flos chrysanthemi* (菊花)

Figure 2.10 *Flos loicerae* (金银花)
Figure 2.11 *Flos fararae* (款冬花)

Figure 2.12 *Flos campsis* (凌霄花)
Chapter 2: Experimental

Figure 2.13 *Flos rosae rugosae* (玫瑰花)

Figure 2.14 *Flos mume* (梅花)
Chapter 2: Experimental

Figure 2.15 Flos buddlejae (密蒙花)

Figure 2.16 Flos rhododendri mollis (鬱羊花)
Figure 2.17 *Flos inulae* (旋覆花)

Figure 2.18 *Flos magnoliae* (辛夷)
Figure 2.19 *Flos rosae chinensis* (月季花)

Figure 2.20 *Flos chrysanthemi indici* (野菊花)
Chapter 2: Experimental

Figure 2.21 *Flos genkwa* (荒花)

Figure 2.22 *Flos daturae* (洋金花)
2.12 Reproducibility of extraction

The experimental procedure was repeated three times for each of the sample to obtain three spectra in order to test for the reproducibility of the extraction method. The relative standard deviation for the peak intensity and that for the peak positions of the three spectra collected for each sample were calculated. The distribution of RSD (%) for the peak position graph and the distribution of RSD (%) for the peak intensities graph were plotted and shown in Figure 2.23 and Figure 2.24 respectively. From the graphs, it can be seen that nearly all peak positions have RSD value below 0.05 % and around 90% of peak intensities have RSD value below 5 %. These results show that the reproducibility of the extraction method is satisfactory.

Figure 2.23 Distribution of RSD (%) for the peak positions with a total of 575 peaks
Figure 2.24 Distribution of RSD (%) for the Peak intensities with a total of 575 peaks
Chapter 3

Application of Library Search Techniques

- Results and Discussion

3.1 Introduction

Library search program is useful in the case where the spectra are not easily
distinguishable from each other. It can reduce the time consumed for comparing the
spectra and increase the reliability of the identification result. However it is
recommended that a visual comparison of the sample and library spectra should be
made before accepting identification.

In the identification of Chinese herbal flowers under study, at least three spectra
were collected for each sample. Library search programs were used for comparing an
unknown spectrum with a set of reference spectra. Two library search techniques
were applied to recognize the spectra. They were Euclidean\(^\text{21}\) and Search Soft
Independent Modeling of Class Analogy (SIMCA)\(^\text{38}\). In the following part the
application of these two techniques on the identification of Chinese herbal medicine
will be discussed.
3.2 Euclidean Search

Before using a Euclidean Search technique, a library database was built by inputting the reference spectra using Library Building Utility. Then Euclidean Search compared the shape of the sample spectrum with the shapes of known spectra in a library, and reported the best matches. The match similarity score was shown in the Euclidean hit list, which would display the 28 highest-scoring spectra from a Euclidean Search.43

3.2.1 Similarity Score of reference spectra

Similarity score is a way of objectively fixing the "degree of resemblance" between two points or between two samples. For Euclidean Search method, similarity score based on the following Euclidean distance40, and the score is automatically calculated

\[D(x,y) = \left(\sum_{i=1}^{N} (x_i - y_i)^2\right)^{1/2}\]

The similarity scores for the reference spectra of the flowers are shown in Table 3.1. The higher the score is, the more closely the sample spectra match to the reference
spectra. Scores of 100 imply that the shapes of the two reference spectra are the same. For each flower in Table 3.1, the similarity scores of all reference spectra are listed. The flower reference spectra with the highest scores are taken out and shown as the hit list (in descending order of the scores) in Table 3.2. We can see that for all flowers the first member in the hit list with score of 100 is the reference sample itself while the second member to the fourth member are the other reference samples in the library.
Table 3.1 the similarity score among the reference spectra

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<th></th>
<th>dx</th>
<th>gjh</th>
<th>hgh</th>
<th>hh</th>
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<th>Hph</th>
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3.2.2 Similarity Score of Known Sample Spectra

After the library databases was built up, a sample could be searched against the library databases. Three known spectra for each sample were obtained and searched against the library databases using Euclidean Search. The similarity score of the known sample to the target reference spectrum were listed in table 3.3.

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Table 3.3 Search results of known sample by Euclidean Method
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### Application of Library Search Techniques - Results and Discussion

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The average similarity score of known sample spectrum to the target reference spectrum were calculated and shown in Figure 3.1 with the standard derivation of the average similarity score shown in Figure 3.2.

It can be seen that 17 out of 21 flowers have average similarity score of above 95 and 4 out of 21 have average score between 90 and 95. All the average scores have relative standard deviation of below 5%.
Figure 3.1 Average similarity score of known sample spectrum to the target reference spectrum

Figure 3.2 Relative standard deviation among scores of the known samples
3.3 Soft Independent Modeling of Class Analogy (SIMCA)

SIMCA is a commercially available software program produced by Perkin-Elmer instruments. It is used to classify an unknown sample in terms of classes.\textsuperscript{44}

SIMCA is built by the idea of Principal Components Model from measurements on a representative group of authentic samples that covers the acceptable range of variation. A sample can be characterized by its principal component score and by the residual for the model of this sample. The principal component scores show whether the sample appears to lie inside the range of the model whereas the residual corresponds to that part of the measurement that cannot be represented by the model. A combination of the scores and the residual are used to calculate the probability that the new sample is within the acceptable range.\textsuperscript{45}

When assigning a sample to one of a number of possible classes, the sample is compared with each model of the class in turn. The sample may fit none of the classes, it may fit only one of the classes, or it may fit more than one of the classes.

Before using the SIMCA program, at least 5 standard spectra for each of the
sample were input. PROCESS was used to calculate the mean and standard deviation of the spectra of the batch. Then a QUANT+ method for each sample class was created and calibrated so that the class can be defined based on the set of spectra. Then the model could be tested by DIAGNOST and the interclass distances, the class distances, recognition and rejection rates, modeling powers and discriminating powers for the variables were calculated in order to check the classes are sufficiently separated.46

The interclass distance $D_{ab}$ is defined as:

$$\frac{(S_{ab})^2 + (S_{bb})^2}{(S_{aa})^2 + (S_{bb})^2}$$

where $(S_{ab})^2$ is the residual variance for the standard of class a when fitted to the model of class b, while $(S_{ba})^2$ is the residual variance for the standard of class b when fitted to the model of class a. $(S_{aa})^2$ and $(S_{bb})^2$ are the residual variances of the standards fitted to their own class models. All the samples are tested against all the models and are summarized in terms of the interclass distances.45
3.3.1 Verification Diagnostic Report of the Reference flowers

Table 3.4 reports the interclass distances, which are the arbitrary distances between each of the class of flowers. The larger the number, the longer is the interclass distance between the two classes, meaning that the classes separate more clearly.
Table 3.4 Verification Diagnostic Reports: interclass distances

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</table>
The recognition and rejection rates are reported in Table 3.5. Take the dx class as an example. 17 out of 17 known spectra of dx were recognized as dx, while 133 out of 133 spectra were rejected and considered to belong to the flowers other than dx in the databases. Hence there is a total of 150 spectra in the library databases (i.e. 17 plus 133). From the diagnostic report, we can see that all 17 dx spectra were assigned to the dx class; therefore the recognition rate for the dx class was 100%. On the other hand, all 133 spectra, which did not belong to the dx class, were rejected by the dx class and therefore the rejection rate of dx class was 100%. For this result, we can see that the recognition rate and the rejection rate are reported 100% indicating good separation of each class of compound and there is no overlapping between the classes. As a result, the library databases could be used for the classification of the flowers.43

After that a set of known spectra which were different from the spectra used in building Quant+ method databases were used to validate the models by using VALID.
Table 3.5 Verification Diagnostic report

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<th></th>
<th>% Recognition rate</th>
<th>% Rejection rate</th>
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<td>100(133/133)</td>
</tr>
<tr>
<td>gjh</td>
<td>100(11/11)</td>
<td>100(139/139)</td>
</tr>
<tr>
<td>hgh</td>
<td>100(7/7)</td>
<td>100(143/143)</td>
</tr>
<tr>
<td>hh</td>
<td>100(13/13)</td>
<td>100(137/137)</td>
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<td>100(144/144)</td>
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<td>100(8/8)</td>
<td>100(142/142)</td>
</tr>
<tr>
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</tr>
<tr>
<td>jh</td>
<td>100(10/10)</td>
<td>100(140/140)</td>
</tr>
<tr>
<td>jyh</td>
<td>100(6/6)</td>
<td>100(144/144)</td>
</tr>
<tr>
<td>kdh</td>
<td>100(10/10)</td>
<td>100(140/140)</td>
</tr>
<tr>
<td>lkh</td>
<td>100(5/5)</td>
<td>100(145/145)</td>
</tr>
<tr>
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</tr>
<tr>
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<td>100(145/145)</td>
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<tr>
<td>xy</td>
<td>100(8/8)</td>
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</tr>
<tr>
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<td>100(4/4)</td>
<td>100(146/146)</td>
</tr>
</tbody>
</table>
3.3.2 Classification of Flowers

CLASSIFY in the SIMCA program was used to test a spectrum against each class to find out if it belonged to that group.\(^{42}\)

A typical Verification Classify Report for each of the twenty flowers which have been correctly classified are shown in pages 53-72. It is noted in the classify software, the critical probability level for correct identification is set at 0.01,\(^ {44,46}\). If the probability of a spectrum to a class is larger than the 0.01 limits, the spectrum will be classified as belonging to the class. If the probability of a spectrum to a class is lower than the 0.01 limits, the spectrum will not be classified to be the class. Take dx on P.53 as an example, dx has a probability value of 0.9677 > 0.01; hence the spectrum was classified as dx.

In addition to the table report, the result can be shown as a graphic representation, which shows the spectrum residuals and model residuals. Spectrum residuals are the residual column, which lists the spectrum residual for each class that is a measure of the lack of fit of the spectrum to the class model. The model residual is the Mahalanobis residual, which is the residual from the hyper box within class space. The distance between the sample spectrum (origin) and the classes is the
combined residual, which is the square root of the sum of the squares of the spectrum residuals and model residuals. The arc is the critical distance. If the combined residual of the spectrum from a class is less than the critical distance, then the spectrum is a member of the class.\textsuperscript{54}

Again, Figure 2.2 on P. 53 confirms that the spectrum is a member of dx.
<table>
<thead>
<tr>
<th>Class name</th>
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Figure 2.2 Classification report of *Flos caryophylli* (丁香)
## Chapter 3: Application of Library Search Techniques – Results and Discussion

### Table: Distance to class

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### Figure 2.3 Classification report of *Flos ericauli* (谷精花)
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Figure 2.4 Classification report of *Flos carthami* (红花)
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Figure 2.5 Classification report of *Flos sophorae* (槐花)
### Chapter 3: Application of Library Search Techniques – Results and Discussion

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![Figure 2.6 Classification report of Flos albizia](image)

Figure 2.6 Classification report of *Flos albizia* (合歡花)
### Chapter 3: Application of Library Search Techniques – Results and Discussion

#### Distance to class

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**Figure 2.7** Classification report of *Flos magnoliae officinalis* (厚朴花)
Chapter 3: Application of Library Search Techniques – Results and Discussion

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Figure 2.8 Classification report of *Flos celosiae cristate* (雞冠花)
### Chapter 3: Application of Library Search Techniques – Results and Discussion

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![Figure 2.9 Classification report of Flos chrysanthemi (菊花)](image)
### Chapter 3: Application of Library Search Techniques – Results and Discussion

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![Figure 2.10 Classification report of Flos loicerae (金銀花)](image-url)
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<th>Probability</th>
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![Figure 2.11 Classification report of Flos fararae](款冬花)
### Chapter 3: Application of Library Search Techniques – Results and Discussion

#### Distance to class

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<th>Probability</th>
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#### Figure 2.12 Classification report of *Flos campsis* (凌霄花)

![Classification report graph](image-url)
## Chapter 3: Application of Library Search Techniques – Results and Discussion

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Figure 2.13 Classification report of *Flos rosae rugosae* (玫瑰花)
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Figure 2.14 Classification report of *Flos mume* (梅花)
## Distance to class

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![Spectral Residuals](image)

**Figure 2.15 Classification report of *Flos chrysanthemi indici* (密蒙花)**
### Chapter 3: Application of Library Search Techniques – Results and Discussion

#### Table 3.1

<table>
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<tr>
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<th>Probability</th>
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#### Figure 2.16

Classification report of *Flos rhododendri mollis* (闹羊花)
# Chapter 3: Application of Library Search Techniques – Results and Discussion

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<th>Probability</th>
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![Figure 2.17](image)

Figure 2.17 Classification report of *Flos imulæ* (旋覆花)
### Table 2.15

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Figure 2.18 Classification report of *Flos magnoliae* (辛夷)
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Figure 2.19 Classification report of *Flos genkwa* (芜花)
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Figure 2.20 Classification report of *Flos chrysanthemi indica* (野菊花)
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</tr>
<tr>
<td>mgh.md</td>
<td>3.251</td>
<td>0</td>
<td>3.251</td>
<td>&lt;0.0001</td>
</tr>
<tr>
<td>yjh.md</td>
<td>8.681</td>
<td>1.328</td>
<td>8.782</td>
<td>&lt;0.0001</td>
</tr>
<tr>
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<td>0</td>
<td>4.546</td>
<td>&lt;0.0001</td>
</tr>
<tr>
<td>lhx.md</td>
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<td>13.12</td>
<td>&lt;0.0001</td>
</tr>
<tr>
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<td>4.71</td>
<td>&lt;0.0001</td>
</tr>
<tr>
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<td>7.92</td>
<td>&lt;0.0001</td>
</tr>
<tr>
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<td>&lt;0.0001</td>
</tr>
<tr>
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<td>0.08681</td>
<td>8.685</td>
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</tr>
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<td>4.432</td>
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</tr>
<tr>
<td>mm.md</td>
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</tr>
<tr>
<td>jh.md</td>
<td>8.275</td>
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<td>8.275</td>
<td>0</td>
</tr>
<tr>
<td>kdh.md</td>
<td>9.44</td>
<td>0</td>
<td>9.44</td>
<td>0</td>
</tr>
<tr>
<td>xy.md</td>
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<td>1.402</td>
<td>9.732</td>
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</tr>
<tr>
<td>hph.md</td>
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<tr>
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<tr>
<td>dx.md</td>
<td>24.35</td>
<td>7.669</td>
<td>25.53</td>
<td>0</td>
</tr>
</tbody>
</table>

Figure 2.22 *Flos daturae* (洋金花)
In the present project, 3 known samples for each flower were used as unknown. As a matter of fact, 55 out of the 60 (91%) samples can be correctly identified by SIMCA classification method, whereas 5 samples were classified as “misclassified” as these spectra fit more than one of the classes. The misclassified samples include *Flos carthami* (hgh), *Flos mume* (Mh), *Flos rhododendri mollis* (Nyh), *Flos daturae* (Ynh) and *Flos chrysanthemi indic* (Yjh).
Table 3.6 SIMCA Classification result of flower samples

<table>
<thead>
<tr>
<th></th>
<th>Number of samples</th>
<th>Number of correct identified sample</th>
</tr>
</thead>
<tbody>
<tr>
<td>DX</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>GJH</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>HGH</td>
<td>3</td>
<td>2*</td>
</tr>
<tr>
<td>HH</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>HHH</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>HPH</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>JGH</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>JH</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>JYH</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>KDH</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>LXH</td>
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<td>3</td>
</tr>
<tr>
<td>MGH</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>MH</td>
<td>3</td>
<td>2*</td>
</tr>
<tr>
<td>MM</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>NYH</td>
<td>3</td>
<td>2*</td>
</tr>
<tr>
<td>SFH</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>XY</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>YH</td>
<td>3</td>
<td>3</td>
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<tr>
<td>YJH</td>
<td>3</td>
<td>2*</td>
</tr>
<tr>
<td>YNH</td>
<td>3</td>
<td>2*</td>
</tr>
</tbody>
</table>

* one sample was classified as misclassified
3.4 Performance Limitation

3.4.1 Euclidean Search Method

In this library search program of this method, the shape of the sample spectrum is compared with that of known spectra in a library, and the similarity scores were calculated and the best match spectra hit list was reported. Only one reference spectrum for each sample is required to build the library database. Moreover, the time for the library search is short and thus it is a convenient method. However, this library search technique can only report the similarly score of the sample spectrum to the reference spectra but cannot classify the sample spectrum. For the case, where the similarity scores of the sample spectrum to two reference spectra are highly similar, it is difficult to identify the sample spectrum.

3.4.2 SIMCA

For the SIMCA, it requires more than 5 spectra for each sample and in order to have better recognition results, more spectra would be input into the library databases. Therefore for those unknown with small number of available samples may not produce satisfactory results with this technique. Further, the time for building up library and perform library search using this technique is longer than that using Euclidean method. Nevertheless, this technique has a higher recognition power and it
can clearly classify the sample spectrum to a reference class. It is more objective and easier to be understood by user.
3.5 Conclusion

On the present research, 64 samples of 21 species of flowers were collected and extracted by the same solvent system, which included some simple and convenient operation steps.

The flowers samples were identified by using two library search techniques, namely, Euclidean Search method and SIMCA classification method. Two library databases were built according based on the spectra collected from the flowers.

The Euclidean Search Method successfully identifies the 21 flowers. 17 out of the 21 flowers have highest similarity scores above 95 while 4 out of the 21 flowers have average scores between 90 and 95. The four flowers are Flos chrysanthemi (Jh), Flos loicerae (Jyh), Flos rosae rugosae (Mgh) and Flos rosae chinensis (Ygh). And all the average scores have relative standard deviation below 5%.

As we can see from Table 3.2 all the similarity scores of the second member in the hit list are below 90 while the average scores of known sample spectrum to the target reference spectrum are all over 90 with the highest relative standard deviation below 5%. Therefore when a sample spectrum has a similarity score to a reference
sample of over 95 it can be concluded that the sample and reference spectra are similar. For the similarity score between 90-95, there is a possibility that the sample and the reference spectra are similar, however for the similarity score below 90, there is highly probable that the sample spectra and the reference spectra are different. Hence, when the similarity score are below 95 other method for identification is required.

For the SIMCA classification method, the program can clearly classify the sample spectrum to a reference class. 55 of the 60 samples (91.7%) could be identified correctly while 5 samples (8%) were classified as misclassified. They are one sample of *Flos carthami* (hgh), *Flos mume* (Mh), *Flos rhododendri mollis* (Nyh), *Flos daturae* (Ynh) and *Flos chrysanthemi indic* (Yjh).

It is thus suggested that Euclidean method be used to identify an unknown sample first, since for the Euclidean method, only one spectrum from the unknown is required. For the case when the sample has the highest similarity score of below 95, the sample needs be identified by the SIMICA classification. As the two methods can successfully identify different flowers, these two methods could complement each other.
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