CHEMOMETRIC DISCRIMINATION OF BLEACHED AND DYED HUMAN SCALP HAIR USING ATTENUATED TOTAL REFLECTANCE INFRARED SPECTROCOPY

NURUL ASMA SALSABILA BINTI MOHAMAD ALIAS

UNIVERSITI TEKNOLOGI MALAYSIA

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NURUL ASMA SALSABILA BINTI MOHAMAD ALIAS

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To my late father, Mohamad Alias Mohamad Yunus and my everything, Aziah Mohd Shah Baki

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ABSTRACT

The range of products, different formulation, and variables used in cosmetic treatments hold out great potential for forensic identification of hair evidence although in reality little of that potential is realized due to preferences on DNA testing and lack of analytical chemistry expertise among forensic examiners. It is therefore of interest to produce a rapid data acquisition technique that can classify cosmetically treated human hair for forensic application. Six female donors with natural black hair underwent a series of cosmetic hair treatments namely bleaching and dyeing. The following hair strands were collected; natural (control), bleached, day-1 dyed hair/ week 0, week 2, week 4, week 6 and week 8. Statistical interpretation of the triplicate absorbance readings of 126 hair samples, determined using ATR-FTIR was used to classify the type of treatments, the two different brands and weekly intervals of collected hair samples. A wavenumber region of hair protein variability from 1750 to 800 cm^{-1} was selected for pattern recognition analysis, Principal Component Analysis (PCA) and Hierarchal Cluster Analysis (HCA). PCA provided a satisfying classification based on the types of cosmetic treatments, brands as well as weekly intervals of hair, and permitted up to more than 90% amount of variance, indicating the reliability and validity of the model. Results from HCA complemented the deduction. This present study sheds light in proposing the use of ATR-FTIR combined with chemometric analysis for a simple and accurate classification technique of cosmetically treated human scalp hair which can be incorporated into a forensic hair screening protocol.

ABSTRAK

Rangkaian produk, formulasi yang berbeza dan pembolehubah dalam penggunaan rawatan rambut kosmetik mempunyai potensi untuk proses identifikasi bukti rambut forensik walaupun dalam realiti potensi itu tidak disedari kerana keutamaan pada ujian DNA dan kekurangan pakar kimia analitikal dalam kalangan pemeriksa forensik. Justeru itu, kajian ini berminat untuk menghasilkan suatu kaedah pemerolehan data yang pantas dan berupaya untuk mengklasifikasikan rambut manusia yang telah melalui rawatan kosmetik bagi tujuan aplikasi forensik. Enam orang subjek wanita yang memiliki rambut asli berwarna hitam telah melalui suatu siri rawatan kosmetik rambut iaitu pelunturan dan pewarnaan. Berikut merupakan rambut yang telah dikumpul ; asli (terkawal), diluntur, hari-1 diwarna/ minggu 0, minggu 2, minggu 4, minggu 6 dan akhirnya, minggu 8. Tafsiran statistik bagi tiga ulangan bacaan serapan 126 sampel rambut telah ditentukan menggunakan ATR-FTIR untuk mengklasifikan jenis rawatan, dua jenama berbeza dan selangan mingguan sampel rambut yang telah dikumpul. Nombor gelombang mewakili kepelbagaian protein dalam rambut bermula dari 1750 hingga 800 cm^{-1} telah dipilih untuk analisis pengenalpastian corak iaitu Analisis Komponen Utama (PCA) dan Analisis Kelompok Hierarchal (HCA). PCA telah menghasilkan klasifikasi yang memuaskan berdasarkan jenis rambut yang telah melalui rawatan kosmetik, jenama produk serta selangan mingguan dan membenarkan sehingga lebih daripada 90% jumlah varians menunjukkan kebolehpercayaan dan kesahihan model sementara HCA melengkapi deduksi tersebut. Kajian ini telah mencadangkan penggunaan ATR-FTIR bersama analisa ‘chemometric’ untuk menghasilkan suatu teknik pengklasifikasian yang ringkas dan tepat bagi sampel rambut kepala manusia yang telah dirawat dengan kosmetik sebagai protokol forensik untuk pemeriksaan rambut.

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LIST OF ABBREVIATIONS

.XLS	-	Microsoft Excel file format
2D	-	2 Dimensional
3D	-	3 Dimensional
ATR	-	Attenuated Total Reflectance
ATR-FTIR	-	Attenuated Total Reflectance - Fourier Transform Infrared
cm	-	centimetres
cm^{-1}	-	Reciprocal centimetres
DNA	-	Deoxyribonucleic Acid
E.g.	-	Exempligratia
etc.	-	Et cetera
FTIR	-	Fourier Transform Infrared
HCA	-	Hierarchal Cluster Analysis
HPLC	-	High Performance Liquid Chromatography
i.e.	-	In essence
Inc.	-	Incorporation
IR	-	Infrared
PCA	-	Principal Component Analysis
PCs	-	Principal Components
PC1	-	First principal component
PC2	-	Second principal component
PC3	-	Third principal component
pH	-	Potential of hydrogen
R groups	-	group in which a carbon or hydrogen atom is attached to the rest of the molecule

SEM	-	Scanning Electron Microscope
TLC	-	Thin Layer Chromatography
USA	-	United States of America
UV	-	Ultraviolet
UV-Vis	-	Ultraviolet-Visible
Vol.	-	Volume
Viz.	-	Videlicet

LIST OF SYMBOLS

C	-	Carbon
H	-	Hydrogen
KBr	-	Potassium Bromide
O	-	Oxygen
S	-	Sulphur

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CHAPTER 1

INTRODUCTION

1.1 Research Background

The field of forensic science is generally defined as the application of scientific approach in legal issues (Nordby, 2005), encouraging the advancement of scientific methods and procedures to facilitate individualization since cases with diverging circumstances are commonly encountered. Evidence, particularly biological specimens, retrieved from the crime scene are most likely affected by the environment (Brandes, 2009). Trace evidence transferred during a crime forms an integral part of a forensic investigation as it may be the significant evidence associating or acquitting an individual to a crime (Barton, 2011).

Apart from blood, human hair is one of the most transferable biological specimens and often found in a large amount (Brandes, 2009). In principle, a person shed approximately 50 to 100 hair strands per day (Deedrick, 2000), making it a common evidence recovered at crime scenes. Due to its rigidity, flexibility as well as durability (Velasco, 2009), hair forms a reasonably good piece of physical evidence. Generally, the information that could be obtained from a single strand of hair includes DNA profile, hair pigmentation, toxicity, and characteristics (e.g. hair colorant or treatments as well as the possible race/ethnicity) (Tobin, 2005). However, the process of acquiring DNA from hair is always subjected to degradation, contamination, extremely costly, and does not always generate successful results, especially in the absence of follicles (Manheim, 2015). Considering instances wherein hairs are found without their follicles, rendering difficulties for extracting DNA, they are classified as the class characteristic evidence (Saferstein, 2011).

Microscopic examination of hair may reveal forensically important information *viz.* color, thickness, shape, race, somatic origin, as well as the method of removal i.e. either forcefully or naturally (Barton, 2011). However, interpretation of the results relies largely on individual expert interpretation that may vary from one another (Manheim, 2015), "owing to a lack of a uniform reference for identifying the specific microscopic characteristic seen in a study hair" (Barton, 2011). In this context, analyzing the chemical compositions of hair, especially the dyed ones using non-destructive analytical instruments such as Fourier Transform Infrared (FTIR) for revealing forensic information has been suggested (Panayiotou and Kokot, 1999). Considering the current trend that involves a myriad of hair treatments (e.g. coloring, bleaching, straightening and perming) (Guerra-Tapia and Gonzalez-Guerra, 2014), as well as the prevailing environmental pollutions (Sporkert *et al*., 2012) that may influence chemical decompositions, continuous researches on such chemical decompositions acquire forensic consideration.

Hair evidence treated with chemical e.g. bleaches or dyes may increase its individuality by providing unique characteristics for criminalistics assessment (Brandes, 2009). Robertson (1999) has classified hair dyes into three main categories namely temporary dyes, semi-permanent and permanent. Ever going development of products and techniques in hair cosmetic treatments may alter the evidential value of hair in terms of morphology (Dias, 2015), chemical composition and its ability in storing the history of the substance of abuse (Cuypers *et al.,* 2014; Crunelle *et al*., 2015). In an instance, bleaching (or also known as oxidation treatment) is reported to alter the structure of cysteine in hair (Kuzuhara *et al*., 2013). Hence, analyzing hair as an evidence may throw light to forensic investigators by providing valuable clues for narrowing down the search.

Currently, the use of chemometric techniques such as Principle Components Analysis (PCA) and Hierarchal Cluster Analysis (HCA) for enabling discriminations of materials has been acquiring popularity (Pilatti *et al*., 2017; Myron *et al*., 2017). In forensic science, such an application has been referred to as forensic provenancing (Kreitals and Watling, 2014). Such chemometric techniques can be especially useful when dealing with populations that exhibit limited genetic divergence with indistinctive boundaries (Alacs *et al*., 2010). As for hair analysis, the use of chemometric techniques has also been reported for chemically treated hair (Barton, 2011; Brandes, 2009; Panayiotou and Kokot, 1999). Considering a great deal of variations in hair treatments, continuous assessments in this aspect may prove useful.

1.2 Problem Statement

Hair remains one of the most important evidence recovered at crime scenes. Although DNA analysis would provide individualization, the fact that in many instances the hair strands are recovered without follicles, analyzing them for DNA profiling may prove problematic (Barton, 2011). Because the use of chemical treatments such as dyes and bleach has been acquiring considerable popularity in the population (Guerra-Tapia and Gonzalez-Guerra, 2014), and may denote certain cults or social groups, characterizing the microscopic traits of hairs such as its morphology and presence of dyes (Dias, 2015), may be useful for narrowing down the search for suspects, an important clue for forensic investigators. The fact that many different types and brands of hair dyes, constituting varying chemical compositions, have been continuously introduced into the market, continuous assessment on chemical characterization of hair *in vivo* proves necessary. In addition, continuous exposure of treated hairs towards the environment, as well as the natural human biological processes may lead to variations in the chemical decomposition of such hairs (Wong, 1972). Hence, this present research that investigated the changes in the composition of varying functional groups between the natural hairs (control) with that of bleached and subsequently dyed using two different brands of Copper hair dyes, for enabling forensic characterization using PCA and HCA, merits specific consideration.

1.3 Objectives and Hypothesis

Using Attenuated Total Reflectance-Fourier Transform Infrared (ATR-FTIR) coupled with either PCA or HCA, this present research was designed to characterize and discriminate the *in vivo*:

(a) Natural and bleached hairs.
(b) Hairs dyed using two different brands of copper dyes.
(c) Hairs dyed by the two different brands exposed to varying weathering intervals (0, 2, 4, 6 and 8 weeks).

It was hypothesized that utilization of the PCA and/or HCA would provide adequate separations among the different groups of hairs and dyes, suitable for criminalistics assessment.

1.4 Scope of Study

The natural, bleached and dyed human scalp hairs were collected from six female subjects residing in Kajang, Selangor. The subjects were divided into two groups i.e. Group A (n=3) and Group B (n=3), each dyeing their hair using the A and B brands of Copper color dye, respectively. Analysis was then done on hairs for both groups exposed to four different intervals (0, 2, 4, 6 and 8 weeks). Pre-discrimination of the hair samples was done using a compound microscope, while ATR-FTIR with the spectral region ranging between 4000-600 cm^{-1} was used for chemical characterization of the collected samples. The data from the IR spectra were interpreted chemometrically using PCA and HCA.

1.5 Significance of Study

The significance of this present study is to ease the process of discrimination of hair evidence found at crime scenes. This study is proposing a method that allows extraction of the utmost forensic information, particularly human hairs that are subjected to chemical treatments. By analyzing its chemical profiles using the statistical interpretation of IR analysis, a more specific discrimination may be feasible, especially when individualization could not be attempted. For real forensic casework applications, the approach may possibly narrow down the search for suspects, as well as exonerate the innocents.

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