

Forensic analysis of condom and personal lubricants by capillary electrophoresis

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Abstract

Condoms may offer sexual assailants a simple and relatively effective means by which they may remove and dispose of the biological evidence of their contact with the victim. Without this valuable probative evidence, the investigator may need to turn to such alternative forms of physical evidence, such as the residue remaining from the condom lubricant, and any other additional lubricating substances, which may have been used by the assailant. In this study, 68 different condom and personal lubricant samples were analysed using micellar electrokinetic capillary chromatography (MEKC) with ultraviolet absorbance detection. The electropherograms were processed by principal component analysis (PCA) and classified with linear discriminant analysis. This classified 233 samples out of 263 into their correct sample group. An alternative method of classification in which the sample electropherograms were converted to vectors and a correlation was determined by the cosine of the angles between these vectors. This correctly classified 172 samples of the 296. Results indicate that the combination of CE with chemometric data treatment offers the potential of being a rapid and efficient means by which condom and personal lubricant samples may be differentiated. Although this analytical method at present lacks the sensitivity required for sexual assault swab analysis, it is hoped that future developments in instrumentation detection capabilities will permit its use one day as a routine casework tool.

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1. Introduction

In cases of sexual assault, the transfer of biological fluids and materials between the assailant and victim provides investigators with valuable evidence of physical contact between the victim and suspect. However, with increasing public awareness of the identifying properties that exchanged biological fluids present and their high evidential value, particularly that of semen, sexual assailants may seek to avoid such transfers and render the evidence inaccessible. Although

various means may be employed to remove the biological evidence from the victim, one of the simplest methods available to the offender is to employ a condom. However, the use of a condom and/or lubricating substance produces its own associated trace evidence, and the detection and identification of such residues can provide valuable intelligence information as well as potential forensic evidence in court [1].

The trace evidence associated with the use of a condom can originate from the condom, additional use of lubricants or both. The range of condom and personal lubricants available world-wide is considerably diverse, and the components present in a lubricant may vary significantly between brands and even varieties of a particular brand. In general, condom and personal lubricants may be divided into four types: silicone-based, polyethylene glycol (PEG)-based, water-based and oil-based with the silicone-based lubricants

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being the most commonly encountered lubricant on condoms [2]. Condom and personal lubricants may also contain spermicidal agents, flavours, colours and perfumes. In cases of sexual assault, the driving need for a lubricating substance by the assailant can also lead to the possibility of the forensic scientist encountering the use of alternative products, which may be any slippery substance ‘at hand’, such as food oils, moisturizing products or medicinal creams.

Blackledge et al. developed a method to detect the presence of polydimethylsiloxane (PDMS) lubricant and nonoxynol-9 based on Fourier transform infrared spectroscopy [3]. The authors were able to provide discrimination by microscopic analysis of other components including corn starch, talc and silica. Furthermore, chemical ionization mass spectrometry was used to compare the PDMS from different manufactures and detect down to 20 ng of material. In a further study, Blackledge [4] measured the viscosity of PDMS lubricants using diffuse reflectance Fourier transform infrared spectroscopy (DRIFTS) and was able to determine the average chain length of different PDMS polymers. This allowed the possibility to determine if the PDMS recovered from evidence items was consistent with the use of a condom.

Hollenbeck et al. [5] utilized liquid chromatography electrospray ionization mass spectrometry (LC-ESI-MS) and matrix assisted laser desorption/ionization Fourier transform mass spectrometry (MALDI-FTMS) to examine evidence in a sexual assault investigation. The authors developed methods using both techniques to detect the presence of nonoxynol-9 from internal vaginal swabs taken post-coitus, and applied the method to an evidence sample. It was concluded that the method could be used to determine the use of some brands of condoms provided other potential sources of nonoxynol-9 could be eliminated.

Maynard et al. [2] developed a protocol for the analysis of condom and personal lubricants based on a series of instrumental techniques including DRIFTS, gas chromatography–mass spectrometry (GC–MS), liquid chromatography–tandem mass-spectrometry (LC–MS/MS) and pyrolysis GC–MS. The authors developed sequence to determine the presence or absence of the major components of the condom and personal lubricants using a methanol and hexane extract of the same swab. The authors’ approach allowed the discrimination of eleven samples from a total of 50 samples, while the remainder of the samples was separated into 9 groups.

Although these methods provide a significant tool for the detection of lubricants consistent with condom use, the methods require relatively expensive instrumentation. In addition the protocols suggested require the use of multiple techniques and are time consuming. Therefore, there is a need for an inexpensive, simple and robust method for the analysis of trace lubricants. Furthermore, methods for reducing analytical data into manageable dimensions for discrimination purposes would be of benefit. Principal component analy-

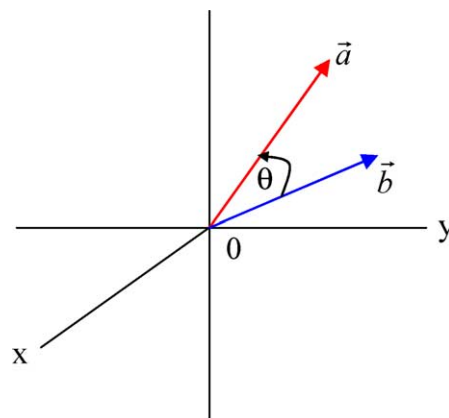


Fig. 1. Vector diagram depicting the position vectors \vec{a} and \vec{b} .

sis (PCA) is one such method. PCA analyzes the covariance structure of multivariate observations [6], and is useful for pattern recognition, particularly where patterns vary within the class to which they belong. Visual interpretation for class determination may be achieved via simple scatter plots of the principal component scores. A linear discriminant analysis (LDA) may also be performed on the principal component scores to determine class membership. LDA calculates the Mahalanobis distance (also known as the squared distance) between observations. Classifications are based on the shortest Mahalanobis distance.

An alternative method is to calculate the similarity of the analytical data of different samples. This may be achieved by converting the electropherograms to vectors [7], such as those depicted in Fig. 1, and compare them using the square of the cosine of the angle between the two vectors:

$$\cos^2 \theta = \frac{(a_1 b_1 + a_2 b_2 + \dots + a_n b_n)^2}{(a_1^2 + a_2^2 + \dots + a_n^2)(b_1^2 + b_2^2 + \dots + b_n^2)} \quad (1)$$

where a_1, a_2, \dots, a_n represent the values of the variables 1 to n for the matrix a , respectively and b_1, b_2, \dots, b_n represent the values of the variables 1 to n for the matrix b , respectively.

The numerical value produced using this method forms the correlation value, and is an easily interpreted ratio value between 0 and 1. Therefore, two samples composed of identical variables (i.e. possessing the same profile) will produce overlapping matrix vectors. The angle between these matrix vectors would then be zero producing a correlation value of 1. Thus, the closer the value between two samples is to 1, the higher the correlation.

This present study investigated the evidential value of water soluble extracts of various samples of condoms and personal lubricants by capillary electrophoresis, and the subsequent processing of the electropherograms by PCA and linear discriminant analysis for brand determination. The calculation of a correlation value as described above was also investigated as alternative for brand determination.

Table 1
Samples analysed listing assigned sample reference number, sample name and manufacturer or distributor, where available

Sample no.	Sample name	Manufacturer/distributor
1	Wet Stuff Personal Lubricant	Gelworks Pty. Ltd.
2	Joy Jelly Unflavoured Lubricant	Doc Johnson Enterprises, Inc.
3	Ansell Personal Lubricant Sachet, banana	Ansell
4	Ansell LifeStyles Ultra Thin Condoms	Ansell
5	K-Y Liquid Personal Lubricant	Johnson & Johnson
6	Ansell Personal Lubricant	Ansell International
7	Sylk Natural Personal Lubricant	Geneva Marketing
8	General Purpose Lubricating Gel	Nelson Laboratories
9	Durex Excita Ribbed Condoms	London Royal Consumer Products, member of LIG
10	Four Seasons Glow N Dark Condoms	Greenmate Company
11	Four Seasons Water Based Personal Lubricant Sachet (sold with Sample #10)	Greenmate Company
12	Saturn Coloured, Fragrant and Flavoured Condoms (a) Strawberry (b) Orange	L S Rubber
13	Ansell LifeStyles (lubricated with nonoxynol 9)	Ansell International
14	Revel Super Thin and Double Contoured Condoms	Okamoto Industries
15	K-Y Jelly Personal Lubricant	Johnson & Johnson
16	Wet Stuff Gold Personal Lubricant	Gelworks Pty. Ltd.
17	Wet Stuff Water Based Personal Lubricant—passionfruit	Gelworks Pty. Ltd.
18	Wet Stuff Water Based Personal Lubricant—musk	Gelworks Pty. Ltd.
19	Wet Stuff Water Based Personal Lubricant—strawberry	Gelworks Pty. Ltd.
20	Satin Gel Water Based Personal Lubricant	Gelworks Pty. Ltd.
21	Glyde Ultra Special Lubricated Condoms	Glyde USA, Inc.
22	Ansell Flavoured Personal Lubricant Sachet—strawberry	Ansell International
23	Passion Regular Nonoxynol 9 Condoms	Hanarum Rubber Tech.
24	Wet Stuff Water Based Personal Lubricant—banana	Gelworks Pty. Ltd.
25	Romantique Lubricant—ravishing raspberry	Biotech International Ltd.
26	Four Seasons Studded Condoms—ultra sensitive	Australian Therapeutic Supplies Pty. Ltd.
27	Four Seasons Coloured Condoms—ultra sensitive (blue)	Australian Therapeutic Supplies Pty. Ltd.
28	Four Seasons Black Coloured Condoms—ultra sensitive	Australian Therapeutic Supplies Pty. Ltd.
29	Four Seasons Water Based Personal Lubricant	Australian Therapeutic Supplies Pty. Ltd.
30	Four Seasons Strawberry Flavoured Condoms—ultra sensitive	Australian Therapeutic Supplies Pty. Ltd.
31	Four Seasons Chocolate Flavoured Condoms—ultra sensitive	Australian Therapeutic Supplies Pty. Ltd.
32	Saturn Nonoxynol-9 Lubricated Condoms	Novus Health Industries
33	Four Seasons Water Based Personal Lubricant—banana flavoured	Australian Therapeutic Supplies Pty. Ltd.
34	Anal Lube	Doc Johnson Enterprises
35	Superlube Premium Grade Personal Lubricant	Wild Nights
36	Cinnamon Motion Lotion	Doc Johnson Enterprises
37	Wicked Water Based Personal Lubricant	Wicked Whims
38	Climax Gel	Claredale Distributors
39	Satin Gel—musk mystique	Gel Works Pty. Ltd.
40	Ben Dover's Original Lube	Doc Johnson Enterprises
41	Satin Gel—banana bliss	Gel Works Pty. Ltd.
42	Wet Stuff Secrets	Gel Works Pty. Ltd.
43	Sax Lubricated Condoms	Unknown
44	Mount Condoms	Unknown
45	WET—wine grape flavoured lubricant	Wet International
46	WET—red apple flavoured lubricant	Wet International
47	WET—seedless watermelon flavoured lubricant	Wet International
48	WET—Kiwi strawberry flavoured lubricant	Wet International
49	Moist Personal Lubricant	Pipedream Products
50	Body Heat—pina colada	Pipedream Products
51	Probe Personal Lubricant	Davryan Laboratories, Inc.
52	Elbow Grease Quickie	B. Cumming
53	Wet Lube Personal Lubricant	Australasian Adult Product Distributors
54	Eros Super Concentrated Body Glide	pjur Group, Germany
55	Body Heat—peaches and cream	Pipedream Products
56	Ansell Aloe Vera Personal Lubricant	London Royal Consumer Products
57	Durex Select Coloured, Exotic Flavoured Condoms—orange	Ansell International
58	Naturals Shampoo with Chamomile for Fine Hair	Colgate-Palmolive
59	Naturals Conditioner with Chamomile for Fine Hair	Colgate-Palmolive
60	Peppers Resort Complimentary Shampoo	Unknown

Table 1 (Continued)

Sample no.	Sample name	Manufacturer/distributor
61	Peppers Resort Complimentary Body Lotion	Unknown
62	Rosken Skin Repair Dry Skin Cream	Warner Lambert Consumer Healthcare Pty. Ltd.
63	Softwash Liquid Hand Wash—almond milk with vanilla	Colgate-Palmolive
64	Avon SPF 30+ Sunscreen	Avon Cosmetics Ltd.
65	UTS Ladies Toilet Liquid Handwash Soap	Unknown
66	Durex Fetherlite Condoms	London Royal Consumer Products
67	Ansell LifeStyles Ribbed Condoms	Ansell International

2. Experimental procedures

2.1. Instrumentation

All experiments were conducted using an Agilent Capillary Electrophoresis (Agilent Technologies, Germany) with UV–vis detection system. An applied voltage of 30 kV was used, with a capillary cassette temperature of 25 °C. Pre-conditioning of the capillary was performed for 3.5 min with buffer prior to each injection. Sample introduction was by hydrodynamic pressure injection at 50.0 mbar for 2.00 s. Absorbance was monitored at 200 nm.

The sample analysis was performed using a Polymicro 75.0 µm i.d. fused-silica capillary (effective length 72.5 cm; total length 80.5 cm). One milliliter polypropylene vials (Agilent, Part No. 5182-0567) with polyurethane snap caps (Agilent, Part No. 5181-1512) were used to contain sample solutions for analysis by the CE.

2.2. Reagents

AR grade sodium tetraborate (decahydrate) and sodium dodecyl sulfate were obtained from commercial laboratory suppliers. 18.2 MΩ Milli-Q water generated by a Millipore water purification system was used for all sample, standard and buffer preparations.

2.3. Samples

According to the Therapeutic Goods Administration [8], there were 145 types of condoms and 118 personal lubricants registered for sale in Australia at the time this research was conducted. In addition to this, the widespread use of mail and internet ordering may mean that there are even more varieties of condoms (unregistered with the TGA and unapproved for sale in Australia) and lubricants available to the individual. Due to the large number of condoms and personal lubricants listed, and taking into account that many vary only in shape, size, colour or flavour, a smaller subset of this group was selected. In addition to these products, samples of materials that may be substituted for personal lubricants, such as shampoo and moisturiser, were also examined.

The products sampled were obtained either by personal donation or purchased from adult retail and local supermarket outlets. Table 1 lists the samples used in this study.

2.4. Electrolyte preparation

Stock solutions of 100 mM sodium tetraborate and 100 mM SDS were individually prepared in water. A buffer solution containing 10 mM sodium tetraborate and 30 mM SDS was then prepared from these stock solutions, giving a pH value of 9.25 ± 0.10 . Once prepared, the buffer was degassed and filtered using a 0.45 µm nylon filter.

2.5. Sample preparation

The sample solvent used for both the condom and lubricant sample profile analyses was the 10% (v/v) buffer in water solution (i.e. 10% the concentration of the run buffer). In cases where the sample was not miscible with the solvent the mixture was shaken, allowed to settle and an aliquot taken from the aqueous layer. Samples containing particular matter or whose appearance was cloudy were filtered using a 0.45 µm nylon syringe filter prior to analysis.

Condoms: Using clean scissors and tweezers, the condom was removed from its package, unrolled and the lubricated section (approximately 10 cm of the tip) cut from the remainder of the condom. Both pieces of the lubricated condom tip were again cut in half, and all four pieces placed in a 20 mL scintillation vial. A micro spatula was then used to scrape out any remaining lubricant from the inside of the condom packaging and also placed in the scintillation vial.

Three milliliters of solvent was then transferred to the scintillation vial, capped and shaken by hand to disperse the water and buffer solution (for approximately 1 min). The sample was then sonicated for 2.5 min intervals, shaken by hand for another 10 s, and then returned to the sonicator for another 2.5 min. An aliquot of the condom lubricant extract was then taken from the scintillation vial and placed in a CE sample vial ready for analysis.

Personal lubricants: A 1% (w/v) solution of each lubricant was prepared by directly weighing the appropriate amount of sample into a volumetric flask, adding solvent and shaking to dissolve the sample. The solution was then made up to volume with additional solvent. An aliquot of the 1% (w/v) lubricant solution was then transferred to a 1 mL capillary electrophoresis sample vial for analysis.

Condom and personal lubricant swabs: To assess whether the CE was capable of detecting such small quantities of lubricating material which might be recovered from a swab

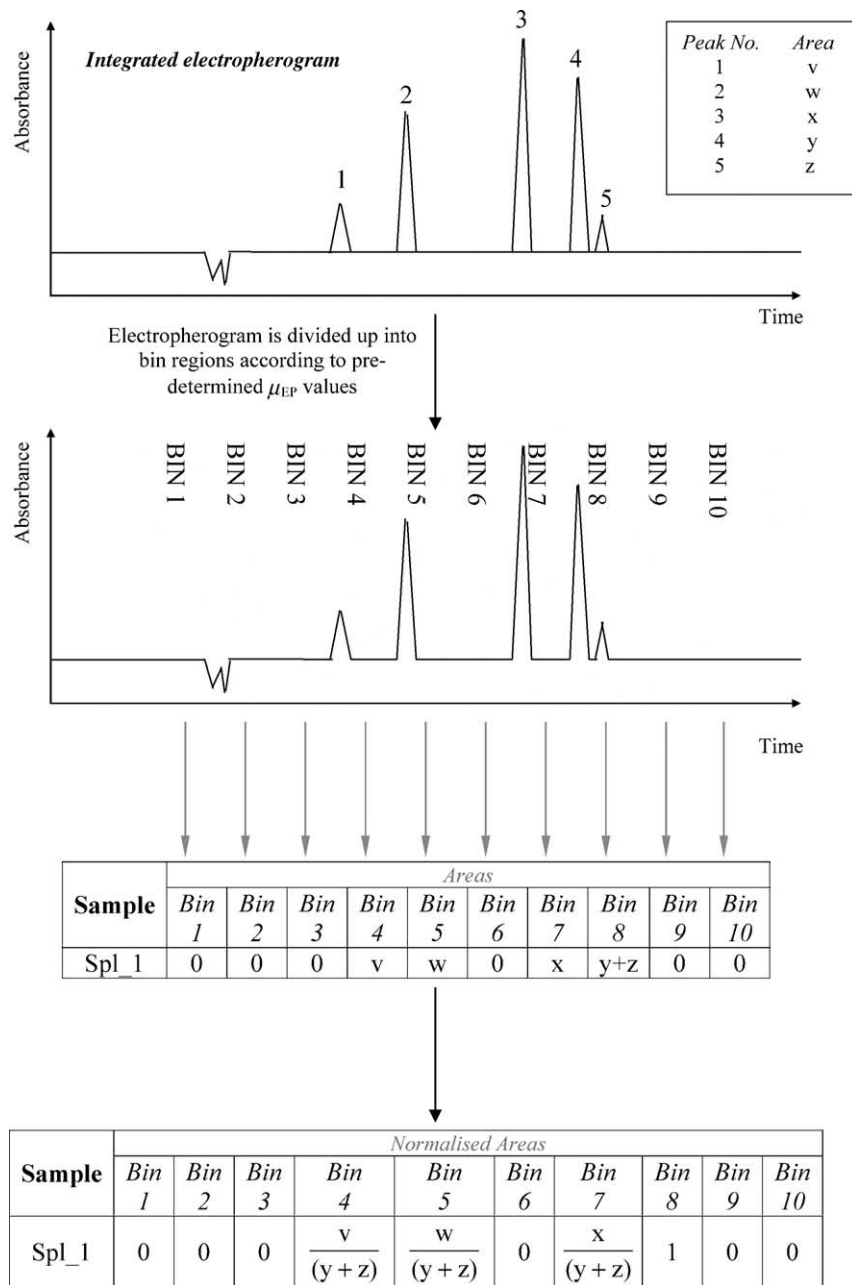


Fig. 2. Data collection and treatment analysis flow diagram.

such as that collected in a sexual assault analysis kit, swab samples from a variety of surfaces were obtained. The swab surfaces analysed included that taken directly from a freshly unrolled condom, personal lubricant deposited on cotton cloth, personal lubricant deposited on human skin (inner arm at the elbow joint) and condom lubricant which was deposited on human skin (inner arm at the elbow joint). Swab samples from the cloth and arm upon which the personal lubricant had been deposited were taken immediately following administration to the area and 30 min afterwards to obtain a rough indication of lubricant persistence.

Swabbing was performed using Dove Flexible Stem Cotton Tips (Accantia Health & Beauty Pty. Ltd.). The use of dry swabs, as well as swab tips moistened with a drop of 10% buffer solution, were examined. In the case of the personal lubricant swabbing, a weighed sample (Sample #42—Wet Stuff Secrets) was spread over a 3 cm × 3 cm area of the surfaces being tested. For the condom lubricant (Sample #10—Four Seasons Glow N Dark Condom), the condom was simply unrolled and the lubricated section sampled.

Swabbing was performed by gently rubbing the cotton tip over a 3 cm × 3 cm surface area. The swab tip was then cut

from the remainder of the stem and placed in a capped test-tube with 1 mL of 10% buffer solution. The sample was then shaken by hand for 1 min, sonicated for another minute and allowed to sit at room temperature for another 10 min. After this an aliquot of the swab extract was then placed in a CE sample vial and analysed. A blank swab was also collected for each surface.

Blank swabs were examined for the presence of extraneous peaks. These peaks were then subtracted from the sample swabs with similar effective mobility values to ensure that the features detected by the data treatment methods possessed minimal sources of background interference.

2.6. Data treatment

The peak areas in each of the electropherograms were calculated using the integration function of Chemstation software (Rev. A.08.03 [847]). Based on the calculated effective mobility values, the electropherogram was divided into 10 bins or data regions, into which each of the peaks were assigned and the peak areas summed. The data for each bin was then normalised according to the bin of greatest value (refer to Fig. 2).

PCA was performed on each of the 10 bins using MINITAB software, Release 13.32. The resulting Scree plot (Fig. 3) gives the eigenvalue of each of the principal component transformations. The eigenvalue is a measure of the variability of the data, the greater the eigenvalue the greater the variability. From this plot, it is clear that most of the variability in the data is explained by the first five principal components (approximately 75%). Therefore, the data matrix was effectively reduced from 10 dimensions to 5 while still maintaining 75% of the information.

Classifications were then determined by LDA using these five principal component scores.

The electropherograms were converted to vectors, and the cosine of the angle between the vectors was calculated via an in-house written program. The bin data for each electropherogram profile was compared against all of the remaining sample profiles and tables of correlation values obtained, forming a result matrix of dimensions 263×263 values.

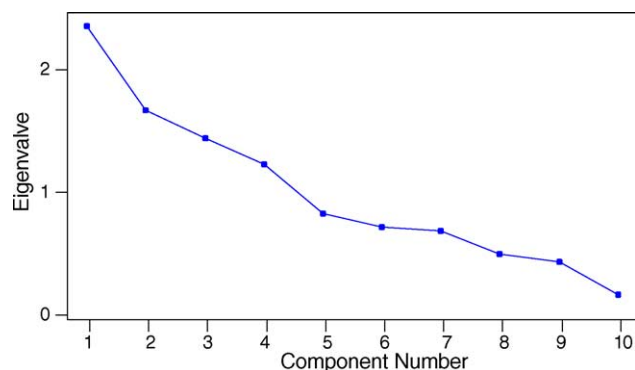


Fig. 3. Eigenvalue (Scree) plot for sample data.

Determination of the correlation “cut-off value” (i.e. how close to 1 the sample profile correlation data value is before a match is declared) was conservatively estimated via averaging of the lowest correlation value for 4 replicate runs of each of the 66 samples, calculated to be 0.9862.

Using this value as the lower limit, a ‘correctly’ matched sample was identified if the other sample replicate profile results were all present as the highest correlation values. A ‘potential misclassification’ would then represent samples where there are correlation values with other product samples, which are higher than one or more of the correct sample group member correlation values. However, these misclassifications are listed only as ‘potential’, as the lower correlation values for that sample group may have been due to the presence of outliers. Samples, which did not correlate with their own group or samples from any other group were considered unidentifiable.

3. Results

Of the 68 samples analysed, two samples, Sample #40 (Ben Dover’s Original Lube) and Sample #54 (Eros Super Concentrated Body Glide) did not produce any detectable peaks in their electropherograms. Sample #29 (Four Seasons Water Based Personal Lubricant) was the only sample to produce a single detectable peak. The remaining samples possessed a minimum of two component peaks (e.g. Figs. 4 and 5).

3.1. Principal component analysis

The principal component and linear discriminant analysis was capable of correctly classifying 233 sample values out of a total of 263, giving a proportion correct value of 88.6%. Of the 68 groups of sample electropherograms analysed, 12 did not produce sets of profiles that could be completely differentiated (a summary of these misclassified observations has been given in Table 2).

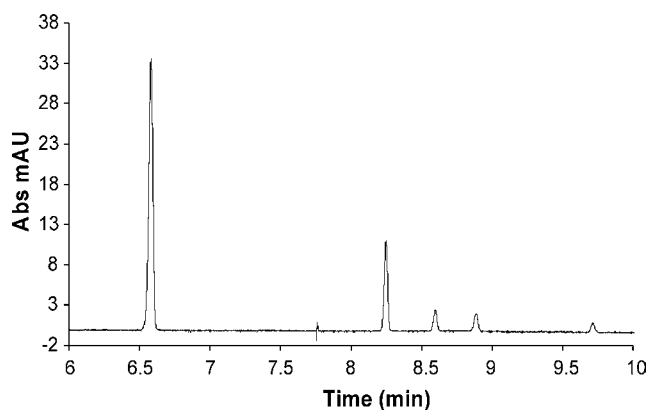


Fig. 4. Example personal lubricant electropherogram (Sample #45—Wet Stuff Secrets).

Table 2
Misclassified samples using PCA and linear discriminant analysis

True sample identity	Predicted sample identity	Fraction of sample replicates misclassified
#3—Ansell Personal Lubricant Sachet	#1—Wet Stuff Personal Lubricant	1 out of 4
#10—Four Seasons Glow N Dark Condoms	#52—Elbow Grease Quickie	1 out of 4
#11—Four Seasons Water Based Personal Lubricant Sachet	#34—Anal Lube	1 out of 3
#18—Wet Stuff Water Based Personal Lubricant (musk)	#20—Satin Gel Water Based Personal Lubricant	2 out of 5
#18—Wet Stuff Water Based Personal Lubricant (musk)	#19—Wet Stuff Water Based Personal Lubricant (strawberry)	2 out of 5
#28—Four Seasons Black Coloured Condoms	#30—Four Seasons Strawberry Flavoured Condoms	1 out of 4
#31—Four Seasons Chocolate Flavoured Condoms	#63—Palmolive Softwash Liquid Hand Wash	1 out of 4
#31—Four Seasons Chocolate Flavoured Condoms	#60—Peppers Resort Complimentary Shampoo	1 out of 4
#32—Saturn Nonoxynol-9 Lubricated Condoms	#23—Passion Regular N9 Condoms	2 out of 4
#33—Four Seasons Water Based Personal Lubricant (banana)	#29—Four Seasons Water Based Personal Lubricant	4 out of 4
#51—Probe Lubricant	#29—Four Seasons Water Based Personal Lubricant	4 out of 4
#54—Eros Super Concentrated Body Glide	#40—Ben Dover's Original Lube	4 out of 4
#61—Peppers Resort Complimentary Body Lotion	#59—Palmolive Naturals Conditioner	4 out of 4
#66—Durex Fetherlite Condoms	#9—Durex Excita Ribbed Condoms	2 out of 4

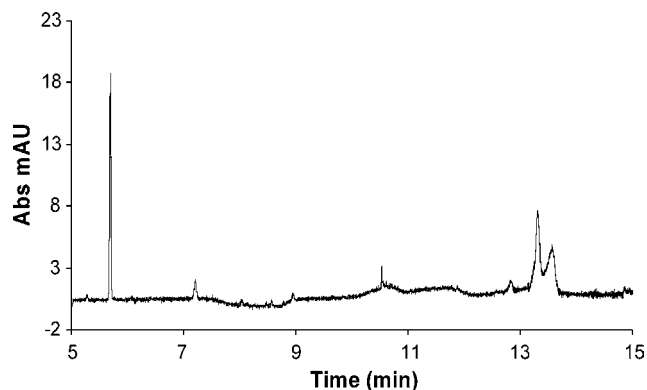


Fig. 5. Example condom lubricant electropherogram (Sample #28—Four Seasons Black Coloured Condoms, ultra sensitive).

3.2. Vector correlation method

Calculation of the correlation value as described earlier produced 172 correct group identifications. Twenty-eight samples could not be correlated to any group within the cut-off value of 0.986. This left 63 samples of 'potential' misclassification. Examples of the data output from calculation of the correlation value for Samples #66 and #67 is given in Tables 3 and 4.

A summary of the sample groups commonly encountered amongst the 'potential' misclassifications is given in Table 5.

Table 3
Example table of first six correlation values for Sample #66 (sample 2, injection 1)—Durex Fetherlite Condoms

Correlation	Sample number and line value
1.000000	s66_2 (Inj. 1)
0.989213	s66_2 (Inj. 2)
0.980833	s10_1 (Inj. 1)
0.977110	s10_1 (Inj. 2)
0.960979	s66_1 (Inj. 2)
0.960144	s66_1 (Inj. 1)

Table 4
Example table of first six correlation values for Sample #67 (sample 2, injection 2)—Ansell LifeStyles Ribbed Condoms

Correlation	Sample number and line value
1.000000	s67_2 (Inj. 2)
0.999767	s67_2 (Inj. 1)
0.999440	s67_1 (Inj. 1)
0.999378	s67_1 (Inj. 2)
0.998113	s14_2 (Inj. 1)
0.995833	s65_1 (Inj. 1)

Inj.: injection.

3.3. Swab analysis

The swabbing and analysis method employed in this study could neither correctly identify condom lubricant directly taken from the condom surface or immediately following skin application. Personal lubricant recovery and identification from the skin and cloth surfaces was successful when sampling took place immediately following application, but no correct identifications were obtained from swabs of these surfaces taken 30 min later. A summary of the results achieved for the swabbing and lubricant persistence study findings using this approach has been given in Table 6.

4. Discussion

4.1. Sample discrimination

The application of this CE method shows some promise for the detection and discrimination of condom and personal lubricants. The production of electropherograms with characteristic features clearly visible to the untrained eye, strongly support its use as a chemical profiling tool. The subsequent treatment of the electropherogram data using either PCA and linear discriminant analysis or calculation of the correlation

Table 5
Misclassified samples using the correlation value

Groups often occurring together in misidentifications	Number of 'potential' misclassifications
#1—Wet Stuff Personal Lubricant	23
#3—Ansell Personal Lubricant Sachet	
#18—Wet Stuff Water Based Personal Lubricant (musk)	
#19—Wet Stuff Water Based Personal Lubricant (strawberry)	
#20—Satin Gel Water Based Personal Lubricant	
#24—Wet Stuff Water Based Personal Lubricant (banana)	
#41—Satin Gel (banana bliss)	
#39—Satin Gel (musk mystique)	2
#41—Satin Gel (banana bliss)	
#11—Four Seasons Water Based Personal Lubricant Sachet	1
#34—Anal Lube	
#21—Glyde Ultra Special Lubricated Condoms	1
#67—Ansell LifeStyles Ribbed Condoms	
#6—Ansell Personal Lubricant	6
#22—Ansell Flavoured Personal Lubricant (strawberry)	
#4—Ansell LifeStyles Ultra Thin Condom	7
#31—Four Seasons Chocolate Flavoured Condoms	
#63—University Hand Wash Soap	
#29—Four Seasons Water Based Personal Lubricant	3
#33—Four Seasons Water Based Personal	
#51—Probe Lubricant	
#9—Durex Excita Ribbed Condoms	3
#66—Durex Fetherlite Condoms	
#45—WET Wine Grape Flavoured Lubricant	9
#47—WET Seedless Watermelon Flavoured Lubricant	
#48—WET Kiwi Strawberry Flavoured Lubricant	
#14—Revel, Super Thin and Double Contoured Condoms	3
#65—University Toilet Hand Wash Soap	
#67—Ansell LifeStyles Ribbed Condoms	
#59—Palmolive Naturals Conditioner	4
#61—Peppers Resort Complimentary Body Lotion	
#9—Durex Excita Ribbed Condoms	1
#52—Elbow Grease Quickie	

value successfully permitted the analyst to gauge the extent to which the various sample profiles differ based on a numerical, non-subjective output value.

Calculation of the correlation value confirmed many of the classifications made using the former approach, strengthening the confidence of correct classification. However, this

method is not as successful for class determination, most likely due to the choice of the threshold correlation value. Without sufficient data on the expected spread of values within a population of samples of a single product, it is difficult to state a value above which samples are considered sufficiently correlated to produce a classification. The number

Table 6
Swab results for personal lubricant (Sample #42) and condom lubricant (Sample #10) on various surfaces

Surface	Swab condition	Identified correctly by PCA linear discriminant analysis?	Correlation correct? (0.986 cut-off)
Personal lubricant on skin for 0 min	Wet	Yes	Yes (correlation 0.998)
	Dry	Yes	Yes (correlation 0.999)
Personal lubricant on skin for 30 min	Wet	No. identified as #16 or #7	Not identified
	Dry	No. identified as #16 or #64	Not identified
Personal lubricant on cloth for 0 min	Wet	Yes	Yes (correlation 0.999)
	Dry	Yes	Yes (correlation 0.999)
Personal lubricant on cloth for 30 min	Wet	No. identified as #16	Not identified
	Dry	No. identified as #16	Not identified
Condom (Sample #10)	Dry	No. identified as #31 and #52	No. identified as #52 (correlation 0.987)
Condom Lubricant (Sample #10) on skin	Wet	No. identified as #63	Not identified

of samples that were not positively classified within the constraints of the approach indicates that further work is required to assist in the interpretation of these correlation values.

4.2. Swab identification

The failure of the principal component and linear discriminant analysis and the calculation of the correlation value to correctly identify some of the swab samples was not unexpected, as the pattern recognition system is based upon a library of data variables obtained from fresh, uncontaminated sample solutions. Ideally such a library will also be composed of samples obtained under a variety of conditions, to reflect the natural changes in the sample over time or when placed in direct contact with reactive compounds selectively adsorbent surfaces.

5. Conclusions

A CE method was developed which was capable of producing differing, and often very individual, sample electropherogram profiles for 66 out of the 68 products analysed. The method involved very few sample preparation steps, employed no organic solvents and was relatively rapid (~20 min per sample). Of the 66 samples that produced electropherogram profiles, the PCA-LDA method correctly classified 233 samples out of a total of 263 into their correct group, and the calculation of the correlation value 172 samples. Of the samples that could not be differentiated, inherent

limitations in the data analysis technique and the similarity in sample formulations could partially account for the lack of complete discrimination ability in the method.

The application of CE to detect and discriminate condom and personal lubricants is of potential use for forensic analysis. However, the inability of this technique to positively identify a known lubricant residue swabbed from a skin or cotton cloth surface only 30 min after application highlights considerable practical limitations of this method, particularly in regards to the analysis of the predicted low trace level concentrations that may be recovered from actual physical sexual assault sample swabs. The potential combination of CE with a mass spectrometer, and future improvements in instrument detection capabilities, may support the use of this method.

References

- [1] R.D. Blackledge, Condom Trace Evidence: A new Factor in Sexual Assault Investigations, May 1996, <http://www.fbi.gov/publications/leb/1996/may964.txt> (accessed 31 May 2002).
- [2] P. Maynard, K. Allwell, C. Roux, M. Dawson, D. Royds, *Forens. Sci. Int.* 124 (2001) 140–156.
- [3] R.D. Blackledge, M. Vincenti, *J. Forens. Sci. Soc.* 34 (1994) 245–256.
- [4] R.D. Blackledge, *J. Forens. Sci.* 40 (1995) 467–469.
- [5] T. Hollenbeck, G. Siuzdak, R. Blackledge, *J. Forens. Sci.* 44 (1999) 783–788.
- [6] K.I. Diamantaras, S.Y. Kung, *Principal Component Neural Networks: Theory and Applications*, Wiley, New York, NY, 1996.
- [7] S. Brown, *Appl. Spectrosc.* 49 (1995) 14A–30A.
- [8] M. Richens, Therapeutic Goods Administration, 15 July 2002, personal communication.