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Forensic Discrimination of White Architectural Paints via ATR FT-IR Spectroscopy and Chemometrics

التمييز الجنائي للدهانات المعمارية البيضاء باستخدام الانعكاس الكلي المنخفض المقترن بالتحليل الطيفي بالأشعة تحت الحمراء والقياس الكيمياء

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Abstract

The present work entailed the comparative examination and discrimination of white architectural paint samples of different brands/manufacturers. The analysis of this evidence can facilitate exhibiting a linkage between the victim, and the crime scene and assist in the reconstruction of the crime scene. Architectural paint traces have evidential value, especially in cases of burglary, acts of vandalism, property crimes, etc. In the present study, a total of 102 samples of 34 distinct brands (3 samples of each brand) of white commercially available architectural paints were purchased and analysed using ATR FT-IR spectroscopy and multivariate analytical tools. The use of visual analysis of FTIR spectral data resulted in 12 undifferentiated/ indistinguishable sample pairs with a discrimination power of 97.86%. Adding PCA and PLS-DA in concert with visual analysis of FTIR spectra resulted in 99.4% (3 sample pairs undifferentiated) and 100% discrimination power, respectively. In conclusion, samples of each brand were completely differentiated using ATR FT-IR spectra subjected to the PLS-DA model. To assess the impact of different substrates on the examination of paint chips, simulated samples were produced on different substrates and the obtained results from the substrates study have been summarized. The ATR-FTIR spectroscopy therefore suggests an objective and rapid approach for the discrimination of white architectural paints for forensic purposes.

Keywords: Forensic sciences, ATR FT-IR spectroscopy, paint analysis, architectural paints, chemometrics, discrimination.

المستخلص

اشتمل العمل الحالي على فحص وتمييز مقارن لعينات طلاء معماري أبيض من علامات تجارية لمُصنعين مختلفين. يمكن أن يسهل تحليل هذا الدليل إظهار الصلة بين الضحية ومكان الجريمة، وبالتالي المساعدة في إعادة بناء مسرح الجريمة. تمتلك آثار الطلاء المعماري قيمة إثباتية، خاصة في حالات السرقة والعبث بالأماكن والجرائم ضد الملكية وغيرها. في هذه الدراسة، تم شراء ما مجموعه 102 عينة من 34 علامة تجارية مختلفة (3 عينات من كل علامة تجارية) من الدهانات المعمارية البيضاء وتحليلها باستخدام الانعكاس الكلي المنخفض المقتن بالتحليل الطيفي بالأشعة تحت الحمراء والأدوات التحليلية متعددة المتغيرات. وأدى استخدام التحليل البصري لبيانات طيف الأشعة تحت الحمراء إلى 12 زوجًا من العينات غير المميزة / غير قابلة للتمييز بقوة تمييزية بنسبة 97.86%. وأدى إضافة تحليل المكونات الرئيسية والتحليل التمييزي باستخدام الانحدار الجزئي المربعاتي الجزئية بالتزامن مع التحليل البصري لأطياف الأشعة تحت الحمراء إلى قوة تمييز بنسبة 99.4% (3 أزواج عينات غير متميزة) و 100% على التوالي. وفي الختام، تم تمييز عينات كل علامة تجارية بالكامل باستخدام الانعكاس الكلي المنخفض المقتن بالتحليل الطيفي بالأشعة تحت الحمراء الخاضعة لنموذج الانحدار باستخدام المربعاتي الجزئية الصغرى- التحليل التمييزي. لتقييم تأثير الركائز المختلفة على فحص رقائق الطلاء، تم إنتاج عينات محاكاة على ركائز مختلفة، وتم تلخيص النتائج التي تم الحصول عليها من دراسة الركائز. وبالتالي، يقترح استخدام الانعكاس الكلي المنخفض المقتن بالتحليل الطيفي بالأشعة تحت الحمراء نهجًا موضوعيًا وسريعًا للتمييز بين الدهانات المعمارية البيضاء للأغراض الجنائية.

الكلمات المفتاحية: علوم الأدلة الجنائية، الانعكاس الكلي المنخفض، التحليل الطيفي بالأشعة تحت الحمراء، تحليل الطلاء، الدهانات المعمارية، الكيمترية، التمييز.



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1. Introduction

White architectural paint is mostly encountered as evidence in forensic investigation purposes owing to the presence of the light shades that are utilized for the architectural finishes. Wright et al. reported that the second important category of paints is architectural paints received in forensic laboratories in North America [1]. The paint fragments are often associated with cases of burglary, homicide, acts of vandalism, and property crimes in distinct forms such as single or multi-layered fragments, smears, chips, droplets, or in the form of stains on different substrates [2,3]. Architectural paints can also be found on various objects which are used to break the building or homes which in turn could be helpful to connect the burglary with the suspect who is holding the tools or implements with these types of traces [4]. However, the traces of paint can be transferred to the victim's clothing and can help reconstruct the events of the crime. The foremost aim of forensic examination of paint evidence is to ascertain their origin and type/brand/manufacturers as well as to compare these traces with the material instigating from the suspect's possession site in criminal investigations. However, in cases, where no comparative material is available, the identification of paint components may provide valuable information about the kind of paint and its brand or manufacturer [5]. The examinations of paint traces are routinely employed in forensic laboratories. The routine forensic examination of paint traces involves the determination of color, layer structure, and its chemical composition [5]. As white paints could not be readily distinguishable based on color, therefore, it becomes necessary to differentiate and characterize this kind of evidence by using various spectroscopic, chromatographic, and other analytical techniques for elemental profiling.

A number of methods are available such as pyrolysis gas chromatography and spectrography [6], Raman spectroscopy [7], infrared spectroscopy [8, 9], Surface-enhanced Raman spectroscopy (SERS) [10], scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), backscatter electron imaging (BSI) and, pyrolysis-gas chromatography (Py-GC) with mass spectrometry (MS), and X-ray analytical techniques [11, 12] for the analysis or examination of paints in the arena of forensic science. The first major all-inclusive study based on the evidentiary value of the architectural paint was conducted by Tippet et al. in 1968 [6]. In the cited study, two thousand samples of paints from houses situated in Wales were intercompared to determine whether the coatings from the different sources were indistinguishable or not. 98% of samples were differentiated by solvent tests and microscopy; however, the remains were examined by using pyrolysis gas chromatography and spectrography. Bell et al. in 2005 [7] emphasized the use of chemometrics with Raman spectroscopy for the discrimination between architectural finishes using a set of 51 "lilac" paints. Muehlethaler et al. 2011 [8] worked on the differentiation of 34 household paint samples of red color by using infrared and Raman spectroscopy. Harroun et al. in 2011 [10] reported the first-ever study on the SERS analysis of exterior and interior wallpaper samples and house paints procured from historic buildings. Nyström, [13] analyzed the spectroscopic measurements of the artists' materials and pigments which are often used as painted wall hangings in southern Swedish from the eighteenth and nineteenth centuries. Wright et al. 2011 published a work on the comparison and discrimination of 964 architectural paint samples that had been acquired from the United States, Canada, and Puerto Rico in the year of 2006 to 2007 [14]. Several techniques were employed in this study such



as stereomicroscope, FTIR (Fourier Transform Infrared) spectroscopy, SEM supplemented with both EDS and BSI, and, Py-GC/MS. Synchrotron radiation-based X-ray analytical techniques were also used to characterize the 16th-century wall paintings [11, 12]. Roberts *et al.* (2013) [9] used a combination of ATR (Attenuated Total Reflectance) FT-IR spectroscopy, Raman spectroscopy, powder X-ray diffraction, and X-ray fluorescence to investigate the thermal decomposition of the paint samples including two-car paints, a clay paint, one matt emulsion, and one metallic paint. The reported work aimed to assess the temperatures at which the paint has been heated, however, distinct temperature markers were detected in the collected ATR FT-IR spectral data.

Among all the reported techniques, FTIR spectroscopy is the most widely used technique for the examination/analysis of artworks, while it is a fast, portable technique and necessitates a very minimum quantity of sample. In addition, its distinct modes of separation, such as ATR, have made this technique useful for the identification and characterization of different types of paints [15–18]. Various studies showed the use of IR spectroscopy which readily detects the type of binder and extenders [19–21], however on the other side Raman spectroscopy is readily used to detect the main pigments [22, 23].

The technique ATR FT-IR (Attenuated total reflectance Fourier transform infrared) spectroscopy has been investigated as a non-destructive and potentially rapid method for the analysis of various traces of evidence such as hairs, fibers, explosives, documents, cosmetics, body fluids, inks, and so on [24,25, 26–33, 34–38]. ATR FT-IR spectroscopy is an effectual non-destructive and non-invasive analytical technique with the benefits of rapid analysis, simple operation, and reduced sample dosage.

Furthermore, the main aim of using multivariate

data analysis or chemometric tools with ATR FTIR spectroscopic methods is to reduce the large dataset to make the easy interpretation of results as in this case the data points generated are large which otherwise creates difficulty in the interpretation of results [39]. Chemometrics methods are widely used with spectroscopic-based techniques in the field of agro-alimentary environmental analyses, analytical chemistry, and forensic sciences. The chemometrics tools such as Principal Component Analysis (PCA) and Partial Least Square-Discriminant Analysis (PLS-DA) are parallely used for a visual approach, however, these approaches are considered more reliable, robust, and efficient than the visual classification approaches [8].

The present work was carried out to differentiate 34 different brands of white architectural paint samples by using the ATR-FTIR spectroscopy subjected to multivariate analytical approaches. Additionally, the effect of simulated case-related substrates on the analysis of white paint has also been investigated.

2. Material and Methods

2.1. Sample collection

Thirty-four different brands of white architectural paint samples were purchased from the paint shops of the Northwestern Indian region. In total 102 samples were collected from 34 brands (3 independent sample of each brand were purchased) of white architectural paints to conduct the reproducibility and intra-brand variation study. Details of all collected samples are listed in Table 1.

2.2. Sample preparation

2.2.1. Neat sample

All collected paint samples were analysed in neat form by introducing a smear of paint on a clean glass slide and then dried overnight at ambi-



Table 1- Details of collected architectural paint samples

Serial Number	Brand	Manufactured By
1.	ASIANPAINTS (Royale Luxury Emulsion)	Crown Packers, GITC, Ankles war 393002.
2.	ASIANPAINTS (APEX ULTIMA Weather proof Exterior Emulsion)	Crown Packers, GITC, Ankles war 393002.
3.	ASIANPAINTS (ACE SPARC Exterior Emulsion)	Redg.Office.6A, Shantinagar Santacruz (East), MUMBAI-400055
4.	ASIANPAINTS (TRACTOR SPARC Economy Emulsion)	Redg.office.6A, Shantinagar Santacruz (East), MUMBAI-400055.
5.	ASIANPAINTS (ACE Exterior Emulsion)	Redg.Office.6A, Shantinagar Santacruz (East), MUMBAI-400055.
6.	BERGER (WALMASTA Antifungal Exterior Emulsion)	Berger House, 129 Street Park Kolkata-700017.
7.	ASIANPAINTS (TRACTOR Emulsion SHYNE)	Redg.Office.6A, Shantinagar Santacruz (East), Mumbai-400055.
8.	NEROLAC (Speed X)	Kansai Nerolac Paints Ltd G.K. Marg, Lower Parel, Mumbai 400013.
9.	SMART (SAMPLAST-Exterior FLAT MATT)	Samsung Fine Chemicals Co. Ltd Samsung Electronic Blog Seoul, Korea 137-857.
10.	ASIANPAINTS (TRACTOR Emulsion Smooth wall finish)	Redg.Office.6A, Shantinagar Santacruz (East), Mumbai-400055.
11.	NEROLAC (BEAUTY Smooth Finish Interior Emulsion)	Kansai Nerolac paints ltd G.K. marg, lower parel, Mumbai 400013.
12.	ASIANPAINTS (APEX Weather proof Exterior Emulsion)	Redg.Office.6A, Shantinagar Santacruz (East), Mumbai-400055
13.	ASIANPAINTS (Royale Luxury Emulsion SHYNE)	Redg.Office.6A, Shantinagar Santacruz (East), Mumbai-400055
14.	ASIANPAINTS (APEX SHYNE Weather proof Exterior Emulsion)	Redg.Office.6A, Shantinagar Santacruz (East), Mumbai-400055
15.	SHALIMAR (Exterior/Super premium 100% Acrylic Emulsion Weather PRO+)	Shalimar paints ltd.
16.	ASIANPAINTS (Apocolite Premium Emulsion)	Redg.Office.6A, Shantinagar Santacruz (East), Mumbai-400055.
17.	SHALIMAR (Superlac stay clean)	Redg.Office.6A, Shantinagar Santacruz (East), Mumbai-400055
18.	SUPERLACPAINTS (Ashiana advance-latex base)	D-39 & 100, B.S. Road Industrial Area, Gharia-bad-201001 (U.P) INDIA
19.	BERGER (WALMASTA Lite Exterior Emulsion)	Berger House, 129 Street Park Kolkata-700017.
20.	SHALIMAR (Interior Acrylic Emulsion)	Shalimar Paints ltd. Fourth Floor, Plot No, 64, Sector 44, Gurgaon-122003, Haryana.
21.	SUPERLACPAINTS (Super Eco)	D-39 & 100, B.S. Road Industrial Area, Gharia-bad-201001 (U.P) INDIA



Table 1 (continued)

Serial Number	Brand	Manufactured By
22.	SUPERLACPAINTS (IMPERIA-Interior Premium Emulsion)	D-39 & 100, B.S. Road Industrial Area, Gharia-bad-201001 (U.P) INDIA
23.	SUPERLACPAINTS (BOSS Advance Plastic Emulsion High Performance)	D-39 & 100, B.S. Road Industrial Area, Gharia-bad-201001 (U.P) INDIA
24.	BERGER (BISON-Acrylic Distemper Interior wall Paint)	Berger House, 129 Street Park Kolkata-700017.
25.	SUPERLACPAINTS (SUPERIA-Exterior Premium Laminate Emulsion)	D-39 & 100, B.S. Road Industrial Area, Gharia-bad-201001 (U.P) INDIA
26.	SUPERLACPAINTS (SILKCOAT-Feather touch Interior Luxury Emulsion)	D-39 & 100, B.S. Road Industrial Area, Gharia-bad-201001 (U.P) INDIA
27.	ACRO PAINTS (ACROSHIELD-Advanced Exterior Emulsion paint)	-
28.	FOREVER PAINTS (4-in-1) Exterior & Interior Primer cum Emulsion	F.C, International Waryana 144013(India)
29.	ASIANPAINTS (Tractor UNO Acrylic Distemper)	Harsh Paint Manufacturing Co. Pvt. Ltd, redg. Of- fice: D-43, Hanuman Nagar, Sanjeevani Marg, Jai- pur-302021.
30.	SUPERLACPAINTS (Classic coat Emulsion Interior & Exterior)	
31.	ASIANPAINTS (APEX ULTIMA PROTEK-Top-coat)	
32.	ASIANPAINTS (TRACTOR ENAMEL)	
33.	BRITISH PAINTS (GLO Advanced enamel)	
34.	ASIANPAINTS (Apocolite GLOSS premium Enamel)	Punjab paint colour & varnish works Pvt. Ltd, 4C, Madan Street, Kolkata-700072.

ent room temperature ($25\pm 5^\circ\text{C}$). Then the samples were scraped out from the glass slides and further analysed by placing the smeared paint on the ATR crystal surface.

2.2.2. On substrates

To study the impact of different simulated substrates on the investigation of paint samples, the following substrates were collected: woollen fabric, white cotton cloth, denim, steel, iron, plastic, wood, tile, glass, wall, watch, gloves, and leather. The clothes were cut into 4.5cm X 4.0cm sized pieces. The paint was equally applied on all the substrates by using a

brush. The applied paint samples were then dried for twenty-four hours at room temperature ($25\pm 5^\circ\text{C}$). Then, the samples were analysed by placing them on an ATR crystal surface with the non-painted part of the same substrate run as the background measurement. Before and after each measurement scan, the ATR crystal was appropriately cleaned by using spectroscopic grade acetone to avoid the unintended chances of cross-contamination.

2.3. Instrumentation

The Spectral data were acquired on the Attenuated total reflectance Fourier transformed infrared



spectrometer [Eco-ATR FTIR, Bruker (Billerica, MA), alpha] equipped with ZnSe crystal and Deuterated L-Alanine Doped Triglycene Sulfate (DLATGS) detector. The data was collected in between the 4000 cm^{-1} - 600 cm^{-1} (mid-IR) range and 4 cm^{-1} resolution with a co-addition of 24 scans. The background measurement was obtained under a parallel set of experimental parameters used for the samples.

2.4 Chemometrics

2.4.1. PCA

PCA is a dimensionality reduction tool for high-dimensional data sets and is consequently used to spot the sample's spectral spatial distribution. It is executed by decomposing or reducing the linear combination of variables into a few principal components. The obtained results with the initial 3 PCs (PC1, PC2, and PC3) were assessed. Nonetheless, the first 2 PCs (PC1, and PC2) were considered the most representative of the analyzed data. Therefore, in this study, we show only the results obtained with PC1 and PC2 [40].

2.4.2. PLS-DA

PLS DA was carried out to develop a model for the classification of paint samples. This approach correlates the dependent (Y) and independent variables (X). The X variables were the spectral matrix; however, the Y variables were the classes of selected paint samples. For the evaluation of PLS regressions, the RMSE, that is, root mean square error, was calculated which quantifies the effectiveness of the calibration model to predict the property of interest in various samples of unknown class [41].

2.5 Spectral Pre-processing

The spectral data was pre-processed before being transported into the chemometric software for statistical interpretation. PCA and PLS-DA chemometric tools were used. ATR correction was subject-

ed to all the obtained FTIR spectra before any other pre-processing methods. For PCA, pre-processing methods included baseline correction, peak area normalization, and the smoothing with Savitzky-Golay algorithm in a polynomial order of three. For the PLS-DA model, non-linear iterative partial least squares (NIPALS) with random cross-validation method algorithm, baseline offset and linear baseline correction, orthogonal signal correction, and de-resolve transform were done.

3. Results and discussion

The representative infrared spectrum of white architectural paint is given in Figure 1. The ATR FT-IR spectra of collected samples were divided into 2 different regions: 1st region (RI)- 4000 to 2800 cm^{-1} and 2nd region (RII)-1800 to 600 cm^{-1} . The region from 1800-600 cm^{-1} exhibits the fingerprint region, and various distinctive peaks were obtained in this particular region and could be supportive in the discrimination of different brands of architectural paint samples. The details of peaks in region 2 (RII) are mentioned in Table 2.

The first peak of RI was obtained approximately in the range of $3620 \pm 50 \text{ cm}^{-1}$ attributed to Talc, Kaolin with OH-stretching band vibrations. Another peak positioned approximately in the range of $3392 \pm 10 \text{ cm}^{-1}$ attributed to n-butylated melamine formaldehyde. The next peak was obtained approximately at 3027 cm^{-1} range corresponding to CH aromatic components. Other peaks were present in the $2952 \pm 10 \text{ cm}^{-1}$ and $2926 \pm 10 \text{ cm}^{-1}$ range corresponding to C-H (CH₂) stretching bands in vinyl toluene and acrylate-modified alkyl resin. The next peak was obtained approximately in the range $2873 \pm 10 \text{ cm}^{-1}$ attributed to n-butylated melamine formaldehyde resin [42]. Table 2



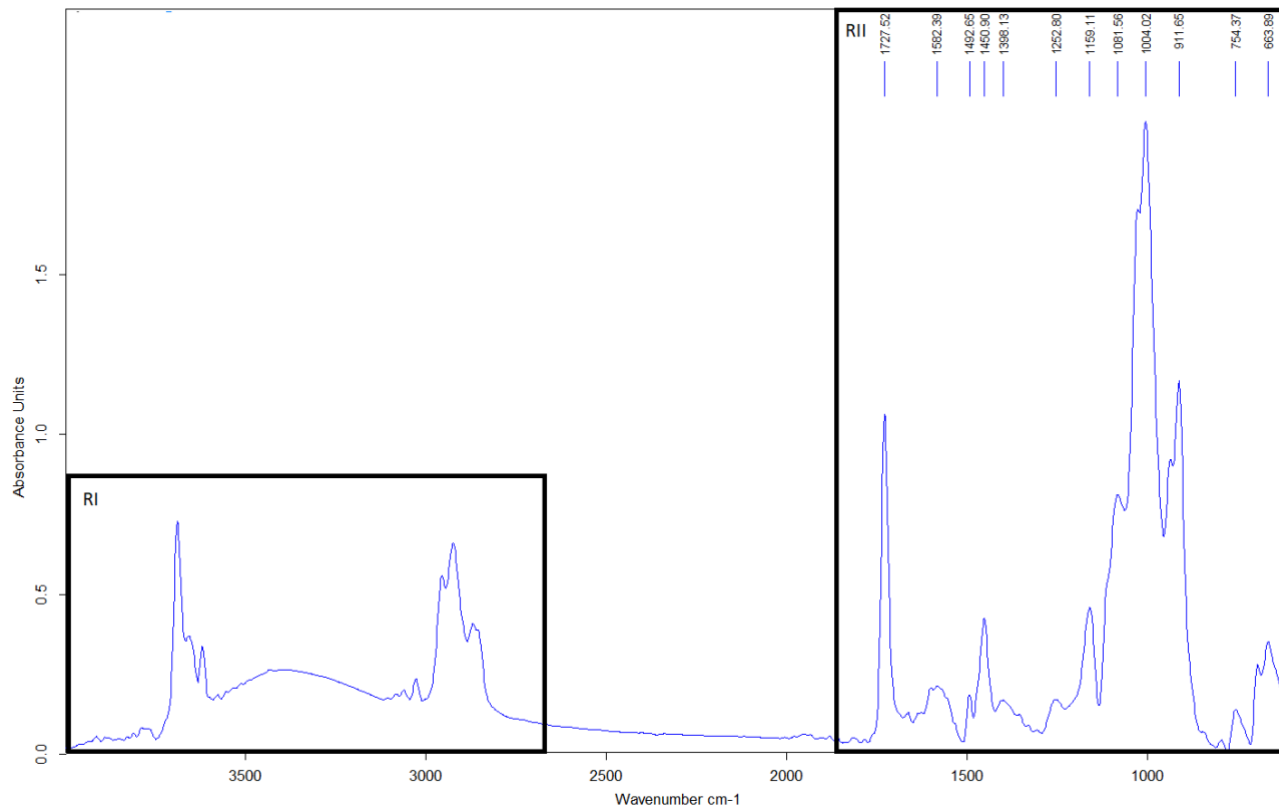


Figure 1- Representative ATR FT-IR spectrum of white architectural paint sample (represented with sample number 1)

Table 2- Classes of compounds identified in architectural paint samples in the range of 1800-600 cm^{-1} [3,8,35,36]

Peaks observed at approximate wavenumbers (cm^{-1})	Components	Functional group
1727	Nitro lacquer, polyurethane, polyester, urethane	Carbonyl bands
1582	Polyurethane, phthalocyanine, scarlet powder	Aromatic stretching
1450	Dolomite, polystyrene, phthalocyanine	CH_2 scissors
1398	Lead white	CO_3^{-2} asymmetric stretching
1253 (1270-1240)	Acrylic resin, polymethylmethacrylate (PMMA).	-
1159	Acrylic resin, phthalate resin, gypsum	SO_4^{-2} asymmetric stretching
1000-1100	Talc, silicate, phthalate resin, Kaolin	$\nu(\text{Si-O})$
911	Kaolin	-
754	Kaolin, Dolomite, polystyrene, aromatic and inorganic components	-

showcases the details of components found in paint samples at specific wavenumbers in the fingerprint region (RII).

Homogeneity, reproducibility, and intra-brand variation study were executed on the collected samples, and through analysis, it was observed



that no visual difference was achieved in the obtained spectra and thus it shows good repeatability, reproducibility, and consistency in the results.

3.1. Discrimination of neat sample

Discrimination of white architectural paint samples was executed by associating their respective ATR FT-IR spectra. The presence or absence of peaks at specific wavenumbers was taken into consideration for discrimination; however, the frequency and shape of the peaks were excluded. The detailed information on peak position with their corresponding wavenumbers is enumerated in Table 3.

Visual inspection of IR spectra suggested that several generated spectra could be successfully discriminated from each other, however, few samples including sample pairs (6 and 8; 3 and 20; 7 and 15; 2 and 17; 19 and 23; 5 and 25; 9 and 22; 9 and 28; 22 and 28; 32 and 33; 32 and 35; 33 and 35) could not be discriminated from each other table 4. Therefore, 97.86% of discrimination power was achieved through visual comparison of FTIR spectra. The chances of recurrent error and subjectivity are more frequent through visual analysis; hence it creates ambiguity in the obtained results. Another point must be noted that visual analysis is only good when analysing a limited number of samples. When the sample size is larger, the chances of error are more frequent which ultimately could lead to the wrong interpretation. Moreover, one-to-one comparison of spectra is also an arduous job for the examiner therefore, it is highly desirable to use multivariate analytical tools to get significant results more objectively.

It is to be noted that this type of analysis holds good for the discrimination of a lesser number of samples. With the increase in sample number, the

chances of error become greater which could lead to biased interpretation of results, and also comparison between spectra becomes an arduous job for analysts. To circumvent aforesaid limitations of visual comparison, the chemometric approach was employed to accomplish objective interpretation of results in the quick time domain, and to reduce the chances of manual errors. The whole purpose of using chemometrics is to process large data sets and to remove the subjectivity of discerning differences in the obtained spectra. It is not feasible to overlay a large number of spectra/ spectral data when building a database and list all the wavenumbers in a table to distinguish the differences in that fashion Table 3.

Discrimination power (DP) as defined by Small-don and Moffat [43]

$$DP = \frac{\text{Total no. of discriminating pair of samples}}{\text{Total no. of possible pair of samples}} \times 100 \dots \text{eq1}$$

Total number of possible sample pairs (n)

$$(n) \frac{n(n-1)}{2} = \frac{34(34-1)}{2} = \frac{1121}{2} = 561$$

Where n denotes the total sample numbers

$$DP = \frac{549}{561} \times 100 = 97.86\%$$

3.2. Discrimination of paint samples using PCA chemometric tool

Before applying the PCA tool, two tests including Kaiser Meyer Olkin (KMO) test and Bartlett's test were performed to confirm the adequacy of the obtained data. How many principal components (PCs) to be picked up was decided by applying the Kaiser Criterion test. The eigenvalues of the principal components are given in Table 5. Another test is Bartlett's test, used to test out the null hypothesis and to locate the correlation among variables. The first



Table 3- Information regarding presence or absence of peaks present in white architectural paint sample.

Sample no.	1800-1700	1660-1500	1500-1400	1400-1300	1300-1200	1200-1100	1100-1000	1000-900	900-800	800-700	700-600
1	✓	-	-	-	-	✓	✓	✓	-	✓	✓
2	✓	-	-	-	✓	✓	✓	✓	✓	✓	✓
3	✓	-	✓	✓	✓	✓	✓	✓	✓	-	✓
4	✓	-	-	-	-	-	✓	✓	-	✓	✓
5	✓	-	-	-	✓	✓	✓	✓	-	-	✓
6	✓	-	-	-	-	✓	✓	✓	✓	✓	✓
7	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
8	✓	-	-	-	-	✓	✓	✓	✓	✓	✓
9	✓	-	-	-	-	-	✓	✓	✓	✓	-
10	✓	-	-	-	✓	-	✓	-	✓	✓	✓
11	✓	-	✓	✓	-	✓	✓	-	✓	✓	✓
12	✓	✓	✓	✓	✓	✓	✓	-	✓	-	✓
13	✓	-	✓	✓	✓	✓	-	✓	✓	-	-
14	✓	✓	-	-	✓	✓	✓	-	✓	✓	✓
15	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
16	✓	✓	✓	✓	✓	-	✓	✓	✓	✓	✓
17	✓	-	-	-	✓	✓	✓	✓	✓	✓	✓
18	✓	-	-	-	-	-	✓	✓	✓	✓	✓
19	✓	-	-	-	-	✓	✓	✓	✓	✓	✓



Table 3 (continued)

Sample no.	1800-1700	1660-1500	1500-1400	1400-1300	1300-1200	1200-1100	1100-1000	1000-900	900-800	800-700	700-600
20	✓	-	✓	✓	✓	✓	✓	✓	✓	-	✓
21	✓	-	-	-	-	✓	✓	-	✓	✓	-
22	✓	-	✓	-	-	-	✓	✓	✓	✓	-
23	✓	-	✓	-	-	✓	✓	✓	✓	✓	✓
24	✓	-	✓	-	✓	✓	✓	✓	✓	-	✓
25	✓	-	✓	-	✓	✓	✓	-	✓	-	✓
26	✓	✓	✓	✓	-	✓	✓	✓	-	✓	✓
27	✓	-	✓	-	-	✓	✓	✓	✓	-	✓
28	✓	-	✓	-	-	-	✓	✓	✓	✓	-
29	✓	-	✓	-	-	-	✓	-	✓	✓	-
30	✓	✓	✓	-	-	✓	✓	✓	✓	✓	-
31	✓	✓	✓	✓	✓	✓	✓	-	✓	-	-
32	✓	✓	✓	✓	✓	✓	✓	✓	-	✓	-
33	✓	✓	✓	✓	✓	✓	✓	✓	-	✓	-
34	✓	✓	✓	✓	✓	✓	✓	✓	-	✓	-

Note: Similar colours in the table indicates non-discriminating samples pairs



Table 4- Details of the non- discriminated samples pairs through visual comparison of FTIR spectra

Serial no.	Non-discriminating sample pairs	Sample pairs
1	6 and 8	1
2	3 and 20	1
3	7 and 15	1
4	2 and 17	1
5	19 and 23	1
6	5 and 25	1
7	9, 22 and 28	3
8	32, 33 and 35	3
Total pairs not discriminated		12

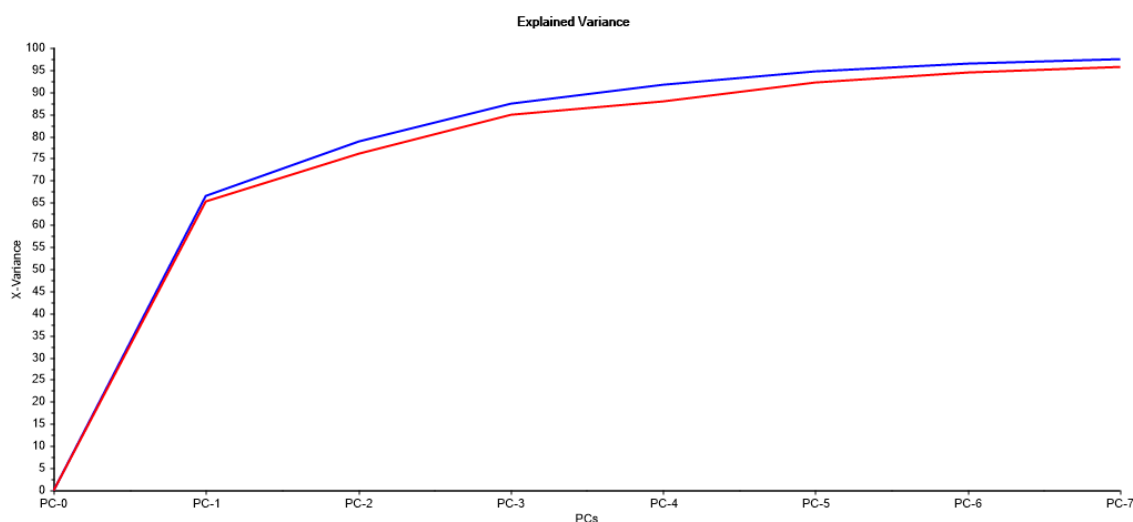
Table 5- Eigen Values

	PC-1	PC-2	PC-3	PC-4	PC-5	PC-6	PC-7
Eigen values	40.34747	7.44097	5.192756	2.517501	1.880482	1.074284	0.624266

six PCs showed an eigenvalue >1 however 7th PC's Eigenvalue was <1 which does not meet the Kaiser criterion as shown in the scree plot Figure 2. As the value of the seventh PC is <1 it could not fulfill the criteria of Kaiser Criterion test. In the present study, initial PCs were selected for the construction of the PCA model. However, the PC1-PC2 combination

plot showed the highest variance in the given data set as demonstrated in Figure 3. The other possible sets of PCs are given in supplementary file as Figure 1 (PC1 vs. PC3) and Figure 2 (PC2 vs. PC3).

All 7 PCs (PC1-PC7) provided 98% (PC1-67%; PC2- 12%; PC3-9%; PC4- 4%; PC5-3%; PC6-2%; PC7-1%) variance; however, initial 2 PCs (PC1-

**Figure 2-** Scree plot- to select PCs

67%; PC2- 12%) opted for the construction of PCA model as the maximum variance was observed with these 2 PCs which accounts 79% of variance in the given data set. 2- Dimensional score plot was constructed for good discrimination of white architectural paint samples from each other; however, all possible sets of PCs (PC1-PC2; PC1-PC3; PC2-PC3) were analyzed but it was shown that PC1 and PC2

showed a higher rate of discrimination. As shown in the PCA score plot; sample numbers 13, 17, 29, 26, 2, 11, 16, 23 existed in positive (+ve) quadrant of PC1 and negative (-ve) quadrant of PC2. Sample numbers 1, 4, 31, 32, 24, 25, 12, 15, 34, 14, 21, 33, and 30 lay on the +ve quadrant of PC1 and PC2. Sample numbers 19, 22, 28, 9, 7, and 27 were distributed among the -ve quadrant of PC1 and the

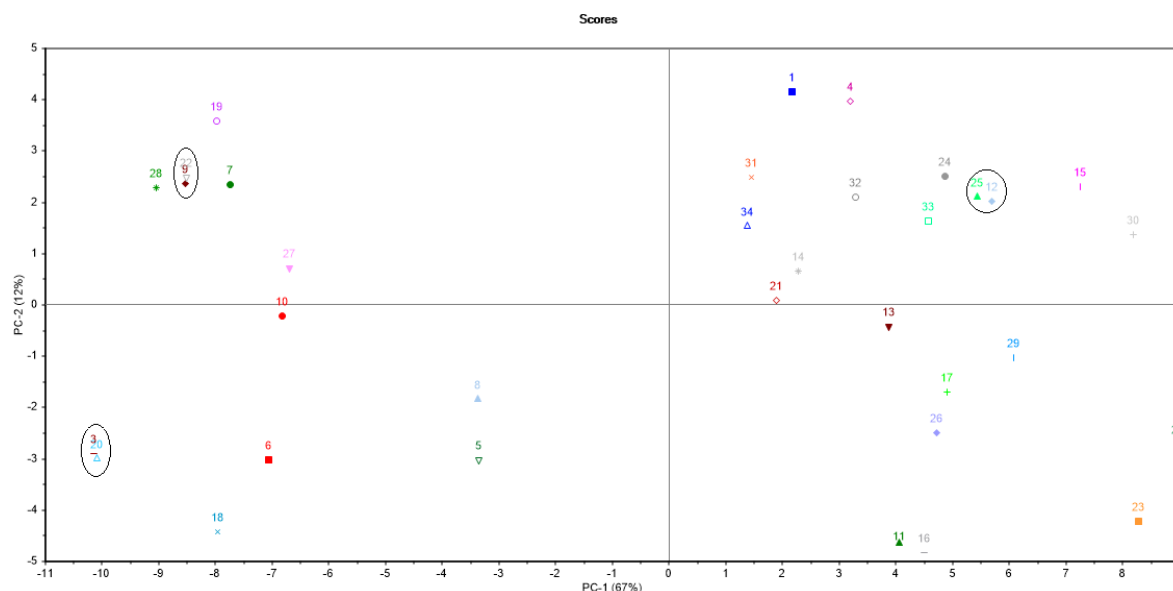


Figure 3- 2D- PCA score plot to discriminate different brands of paint samples

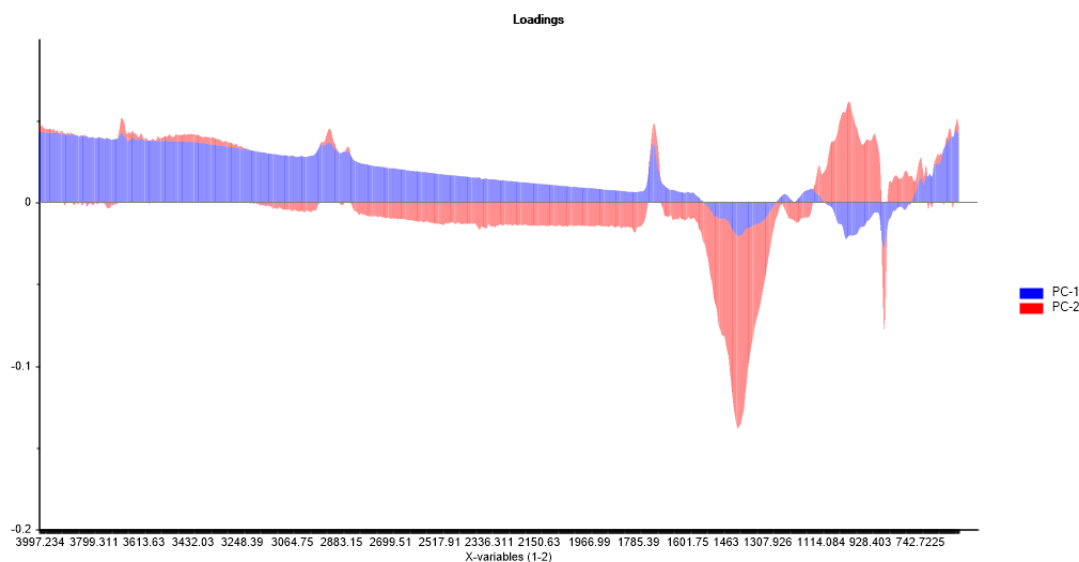


Figure 4- Combined loading plot of PC1 and PC2 to discriminate the paint samples



+ve quadrant of PC2. Sample numbers 10, 3, 20, 6, 8, 5, and 18 dispersed along with the -ve quadrant of PC1 and PC2. The results of PCA suggested 99.4% discrimination power for the discrimination of diverse brands of paint samples (calculated by eq. 1). Figure 4 demonstrates the loading plot of PC1 and PC2. Individual plot of PC1 and PC2 is given in the supplementary file as Figure 3 and Figure 4, respectively. Range from 3997-2840; 1750-1685; and 7777-600 cm^{-1} showed +ve correlation for both PC1 and PC2. Range from 2834-1756 displayed +ve correlation for PC1 and -ve correlation for PC2; range from 1550-1234 cm^{-1} presented +ve correla-

tion for both PC1 and PC2. Range from 1126-885 cm^{-1} exhibited -ve correlation for the PC1 and +ve correlation for PC2. Table 6 shows the undifferentiated sample pairs using the PCA model. The calibration vs. validation plot of PCA model is given in supplementary file Figure 5. This plot provides an indication that how much of the variation in the data is described by the different components. The calibration variance is entirely depend on fitting the calibration data to the model, however, the validation variance is calculated by testing the model on the data which was used to the build the model. The comparison between two set was carried out which

Table 6- Non-discrimination sample pairs using PCA model

S. no	Non-discriminating sample pairs	Sample pairs
1	9 and 22	1
2	3 and 20	1
3	12 and 25	1
Total pairs not discriminated		3

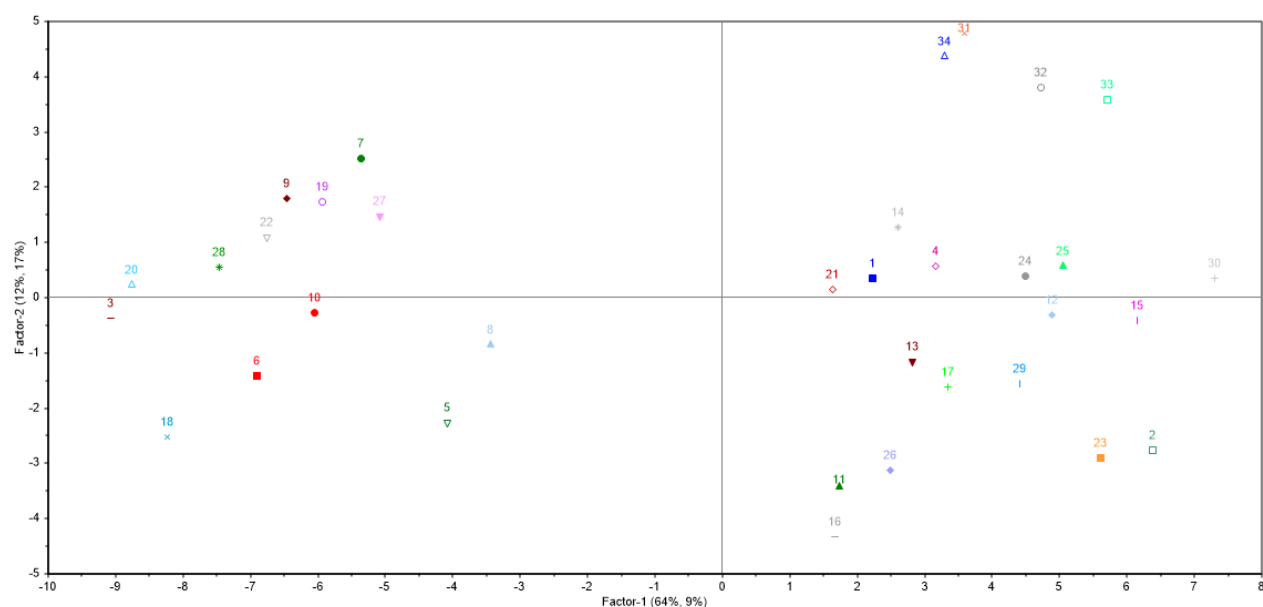


Figure 5- 2D PLS-DA model to discriminate the architectural paint samples of different brands



signifies that explained validation variance is similar to the explained calibration variance which indicates that the calibration and validation data are well fitted.

3.3. Discrimination of paint samples of different brands using the PLS-DA model

The PLS-DA model is a well-acknowledged supervised classification tool and is utilised to get a better discrimination rate than the PCA model. The 2-D plot of the PLS-DA model was generated by using 34 IR spectra obtained from 34 different brands of paint samples Figure 5. To select the number of components, an explained variance plot was constructed. This plot illustrates how much of the total variation in X or Y is described by models including different numbers of components. The total residual variance is computed as the sum of squares of the X- or Y-residuals divided by the number of degrees of freedom.

$$\frac{100 \times (\text{initial variance} - \text{residual variance})}{\text{initial variance}} \quad \text{Eq. 2 [44]}$$

As suggested by the explained variance plot, two factors were selected to construct the PLS-DA model. Factor 1 executed a total 64% of the variations, however, factor 2 demonstrated 12% of overall variations in a given dataset. It was attributed that all 34 brands of architectural paint samples were discriminated from each other. 100% discrimination power was observed using the PLS-DA model. Hence, the PLS-DA

model was considered as a superior model to PCA for the discrimination purposes between samples.

Sample numbers 2, 11, 12, 13, 15, 16, 17, 23, 16, and 29 were dispersed on the +ve axis of factor one and the -ve axis of factor two. Other sample numbers including 1, 4, 14, 21, 24, 25, 30, 31, 32, 33, and 34 were dispersed through the +ve values of factor one and factor two. Sample numbers 7, 9, 19, 20, 22, 27, and 28 were scattered towards the -ve axis of factor one and the +ve axis of factor two. Sample numbers 5, 6, 8, 10, and 18 were diffused down the -ve axis of both factor one and factor two.

Validation (cross-validation) study was carried out through PLS-DA model.

The validation study was conducted on different brands of paint samples to examine the robustness of the PLS-DA model. For the validation study, the cross-validation method was used. In the cross-validation (CV), the same samples were used both for model estimation and testing. A few samples were left out from the calibration data set and the model was calibrated on the remaining data points. Then the values for the left-out samples were predicted and the prediction residuals were computed. The process was repeated with another subset of the calibration set, and so on until every object had been left out once; then all prediction residuals were combined to compute the validation residual variance and Root Mean Squared Error of Prediction (RMSEP). Three paint samples of the same brands were measured

Table 7- Calibration and validation table

	Slope	Offset	RMSE	R-Square
Calibration	0.0887182	15.947432	9.3654089	0.0887182
Validation	0.0263045	17.021772	10.028243	0.0244931



to establish a model across samples and thus it generated three cross-validation segments. Thus, it provided information on the validation results per each cross-validation segment including RMSEP, bias, slope, offset, and correlation. The cross-validation prediction diagnostics were added as a matrix in the validation folder of the PLS-DA model.

The validation results of the PLS-DA model are illustrated in Table 7. Slope, offset, RMSE, and R2 (R-Square) values for both the dataset that validation and calibration data set are given in Table 7. The R2 value exemplifies the relationship among the reference vs predicted samples, however, the R2 value nearer to one advocates the correlation of a stronger degree. The calculated R2 value in the case of the calibration data set was 0.09 and the validation data set was 0.03. The RMSE value intended for the calibration data set was 9.4 and for the validation data set was 10.02. The attained values for the predicted and reference samples are extremely nearer to each

other which demonstrates that the PLS-DA model is adequately robust for the prediction of samples by their respective brands. The slope value for the calibration and validation dataset is 0.09 and 0.02, respectively. The value of offset for the calibration and validation dataset is 16 and 17, respectively. The confusion matrix for the cross-validation study is given in Table I (supplementary file). The confusion matrix is a matrix used for the visualization of classification results from supervised methods. It carries information about the predicted and actual classifications of samples, with each row showing the instances in a predicted class, and each column representing the instances in an actual class [44].

4. Preliminary analysis of white architectural paint samples on different substrates

Traces of deposited paint samples may be encountered from a variety of substrates during crim-

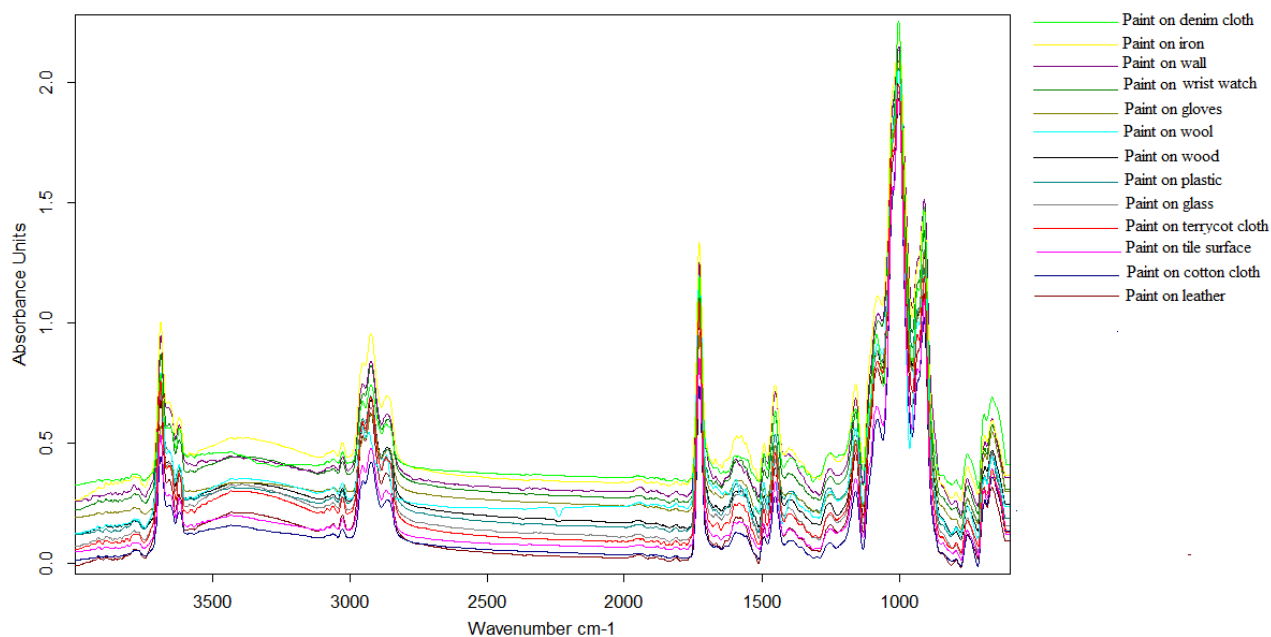


Figure 6- Overlaid ATR FT-IR spectra of Paint samples deposited on different substrates (Represented with sample number 1)



inal investigation. Consequently, the effect of substrate on paint sample analysis was also studied (Figure 6). In the present study, 13 different substrates such as white cotton cloth, plastic, denim, terry cot, wall, glass, watch, wood, wool, tile, leather, gloves, and iron were taken and paint was placed on these substrates, and analyzed by using the above-mentioned procedure (Methodology section). The overlaid FT-IR spectrum of the neat paint sample and the spectra of the deposited paint sample on selected substrates have been shown in Figure 6. Results suggested that all the significant peaks of the paint sample were present on all the selected substrates. Paint is highly viscous and thick therefore; no interference of any substrates (porous or non-porous) was observed in the analysis of paint by using the ATR FT-IR spectroscopy.

ATR FT-IR spectroscopy puts forward the potentiality of non-destructive and on-field, approaches for the analysis of paint traces and possesses disparate advantages over the currently used methods. The major challenge with ATR FT-IR spectroscopy is the inability to detect and identify the traces on various porous substrates. The porosity of the substrates and viscosity of the samples play a vital role in obtaining a good quality spectrum. In case of paint traces, samples are very thick and viscous therefore, no additional effect of substrates was observed on the obtained spectrum. Another well-documented limitation of ATR FT-IR spectroscopy has been deemed problematic when analyzing trace evidence in liquid form. However, in the present study, paint traces were dried first and then analyzed.

5. Conclusion

A rapid and non-destructive method is reported using ATR FT-IR spectroscopy assisted with a chemometric approach for the forensic discrimination of Architectural paint traces. This study revealed that ATR FT-IR in combination with chemometric tools has considerable potential for identification and discrimination of 34 different brands of white architectural paints. The fact is that it is a non-destructive and rapid technique that provides information about the various constituents and is sufficiently able to discriminate architectural paint samples based on their brands/manufacturers. Nevertheless, the significant advantage of ATR FT-IR spectroscopy is its high level of repeatability and reproducibility in the obtained spectra. When the obtained FTIR spectra of white paints were visually/ manually compared, 12 indistinguishable sample pairs out of 561 sample pairs were established, which resulted in a discrimination power of 97.86%. Furthermore, the PCA chemometric tool was applied, which resulted in 99.4% of discrimination power as 3 sample pairs (9 and 22; 3 and 20; 12 and 25) could not be distinguished. However, the PLS-DA tool provided 100% discrimination power as all selected samples were successfully discriminated. The substrate study suggested that all paint samples deposited on different substrates were completely overlapped with the control spectra. Therefore, no influence of any selected substrate was observed on the analysis of paint traces on different substrates.

All-encompassing, ATR FT-IR spectroscopy in combination with multivariate analytical tools has a great potential to entrust facile, rapid, environment-friendly, non-destructive, reliable, and reproducible results for the discrimination of white architectural paint samples. Withal, ATR FT-IR



spectroscopy could be employed for the elimination of samples by comparing them with the samples of the reference data set.

We advocate that further more elaborative studies must be performed on various validation parameters and pertinency of current methodology to evaluate the effects of various other substrates, environmental, and weathering conditions by simulating actual case work conditions on sample analysis. In future, we foresee undergoing further investigations on the applicability of ATR FTIR spectroscopy for the analysis of other brands of architectural paint samples under simulated casework conditions.

Conflict of interest

The authors declare no conflicts of interest.

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