Identification of Gelatin in Dental Materials using the Combination of Attenuated Total Reflection-Fourier Transform Infrared Spectroscopy (ATR-FTIR) and Chemometrics

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ABSTRACT

Gelatin is a multifunctional ingredient widely used in the food and beverage industries. It is also useful in pharmaceutical industry, such as in the manufacturing of dental materials, whether as a main ingredient or an additive. The dental materials traded within Indonesia come from imported goods and local manufacturers. Gelatin is obtained through hydrolysis of cartilages, bones, and skins of cows, pigs and fish. Therefore, the presence of gelatin in dental materials posses critical haram risk for Moslems. This research aimed to examine the presence of gelatin in dental materials using Attenuated Total Reflection-Fourier Transform Infrared Spectroscopy (ATR-FTIR) combined with chemometrics. Gelatin was identified from comparing the infrared (IR) spectrum between samples and standard gelatin of bovine and porcine origins. We combined the IR data with chemometrics through Principal Component Analysis (PCA) and subsequent Soft Independent Modeling of Class Analogy (SIMCA) techniques in order to authenticate the gelatin source. The result showed that 4 out of 49 samples (DM-1, DM-6, DM-18, and DM-27) were detected with gelatin. Based on chemometrics analysis, one sample (DM-6) had similar profile with porcine gelatin. The research highlighted the potential use of combined techniques of ATR-FTIR and chemometrics in authenticating the gelatin source in pharmaceutical products.

1. Introduction

Recently, there is an increasing demand for halal products globally, which not only includes foods and beverages, but also encompasses pharmaceutical products, such as vaccine, drugs and dental materials. A study in Malaysia by Irfanita et al. (2017) detected the gelatin presence in the dental materials that are commonly used in the dental hospitals and dental clinics. Gelatin is a mixture of proteins obtained from bone or skin of cows, pigs, or fish through hydrolysis.(GMIA. 2012) Gelatin from pigskin is clearly haram for Moslims, while those derived from cows can be lawful or syubhat (doubtful), depending on the method of the slaughtering, whether it is in accordance with Islamic law or not. Gelatin from fish is considered halal. The dental materials sold within Indonesia are supplied by international and domestic producers. According to the article 4 of the Indonesian Law Number 33 of 2014 on Halal Product Assurance, all products that enter, circulate, and traded in Indonesia must be halal-certified. The halal status of dental products traded in Indonesia is still

doubtful, if there is no guarantee from the manufacturer in the form of halal logos or halal certificates.

The methods of gelatin identification in various products have been widely studied by researchers. (Demerhan, et al. 2012; Roswiem and Kesuma. 2018; Raraswati et al. 2011; Sahilah et al. 2012; Tasara et al. 2015) One of them is by using the Attenuated Total Reflection-Fourier Transform Infrared Spectroscopy (ATR-FTIR). Most studies focused on identifying pure gelatin or gelatin in processed foods (Hashim et al. 2010; Hidayatullah. 2014) and drug capsule shells, (Syafiqoh, 2014), but not on identifying gelatin in dental materials. The purposes of this study were to detect the presence of gelatin and authenticate its source from the dental materials found in dental hospitals and clinics by using the combination of ATR-FTIR and chemometrics techniques.

2. Materials and methods

2.1. Samples

The dental materials used in this study were drugs and materials used in dental clinics, laboratories and the dentist's offices in general. The number of samples in this study was 49. Product types include powder, liquid, sponge, gel and paste.

2.2. Instruments

The study used the following instruments: Nicolet™ iS™5 FTIR spectrometer with iD7 ATR accessory (Thermo Scientific, USA), OMNIC software (Thermo Scientific, USA), and incubator.

2.3. Procedures

2.3.1. Materials

Bovine and porcine gelatin were purchased from Sigma Aldrich (St. Louis, Mo USA) as standars. Various dental materials from dental clinics, laboratoriums and hospitals were collected as samples.

2.3.2. Sample preparation

Control samples (pure porcine and bovine gelatins) and samples in powder form were dissolved in deionized water and incubated at 50 °C for 10 minutes, until the solution turned clear. Dental materials samples in the form of liquid, paste or gel, were directly placed on the surface of ATR.

2.3.3. Preparation of homemade dental paste

To ensure the presence of gelatin in dental materials, we prepared homemade dental paste products containing standard porcine and bovine gelatin at concentrations of 5%, 10%, 15% dan 20%. The standard gelatin was mixed with sodium bicarbonate, sodium chloride, and water to form a paste (Irfanita et al, 2017).

2.3.4. Analysis of gelatin in samples with ATR-FTIR

The identification of gelatin in the samples was carried out qualitatively by comparing the FTIR spectra of dental material samples with the spectra of standard porcine or bovine gelatin. All infrared spectra were recorded within the range of 4000-500cm^{-1} with 4 cm^{-1} resolution and 32 scans

2.3.5. Analysis of gelatin source

The IR spectra were subject to Principal Component Analysis (PCA), which is really helpful in classifying objects. The PCA plots were then analysed by Soft Independent Modeling of Class Analogy (SIMCA) method (Branden and Hubert, 2005). By using the SIMCA models that had been built, the identification of gelatin source was carried out on the samples.

3. Results and discussion

3.1. Results

3.1.1. Dental material samples

The samples included 49 dental materials from dental and oral hospital of Universitas YARSI, other dental hospitals and dental clinics in Indonesia. The dental materials were sourced from within and outside Indonesia. The categories of the samples were preventive materials, impression materials, restorative materials, and haemostatic agents. The full list of all samples in this study is shown in Table 1.

Table 1. List of samples

No	Code	Category	No	Code	Category
1	DM 1	Preventive Materials	26	DM 26	Preventive Materials
2	DM 2	Impression materials	27	DM 27	Preventive Materials
3	DM 3	Impression materials	28	DM 28	Preventive Materials
4	DM 4	Restorative materials	29	DM 29	Restorative materials
5	DM 5	Impression materials	30	DM 30	Haemostatic agent
6	DM 6	Haemostatic agent	31	DM 31	Preventive Materials
7	DM 7	Impression materials	32	DM 32	Preventive Materials
8	DM 8	Impression materials	33	DM 33	Restorative materials
9	DM 9	Restorative materials	34	DM 34	Restorative materials
10	DM 10	Restorative materials	35	DM 35	Restorative materials
11	DM 11	Restorative materials	36	DM 36	Preventive Materials
12	DM 12	Preventive Materials	37	DM 37	Preventive Materials
13	DM 13	Preventive Materials	38	DM 38	Preventive Materials
14	DM 14	Preventive Materials	39	DM 39	Preventive Materials
15	DM 15	Restorative materials	40	DM 40	Restorative materials
16	DM 16	Restorative materials	41	DM 41	Restorative materials
17	DM 17	Restorative materials	42	DM 42	Restorative materials
18	DM 18	Preventive Materials	43	DM 43	Preventive Materials
19	DM 19	Retorative materials	44	DM 44	Haemostatic agent
20	DM 20	Retorative materials	45	DM 45	Restorative materials
21	DM 21	Restorative materials	46	DM 46	Restorative materials
22	DM 22	Restorative materials	47	DM 47	Restorative materials
23	DM 23	Restorative materials	48	DM 48	Impression materials
24	DM 24	Preventive Materials	49	DM 49	Preventive Materials
25	DM 25	Preventive Materials			

3.1.2. Infrared spectrum from comparative control (standard)

The comparative controls in this study were gelatin solutions of standard porcine and bovine gelatin. Figure 1 shows the infrared spectra of porcine and bovine gelatin obtained from ATR-FTIR software. The infrared spectra of bovine gelatin had similar patterns with porcine gelatin. There were 4 regions observed as follows: 3700-2400 cm^{-1} (Amide A); 1700 - 1654 cm^{-1} (Amide I); 1600 - 1500 cm^{-1} (Amide II) and 1450 - 570 cm^{-1} (Amide III).

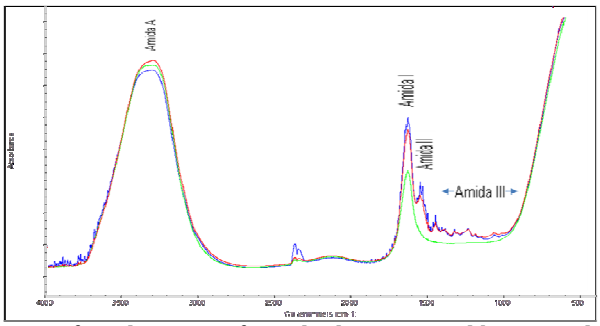


Fig 1. Infrared spectra of standard porcine and bovine gelatin
Note : Red = Bovine gelatin 20%, Blue = porcine gelatin 20%, Green = Water

3.1.3. FTIR Spectra of homemade dental paste

Figures 2a and 2b show the FTIR spectra of homemade dental paste containing gelatin at various concentrations (5%, 10%, 15%, and 20%). The addition of gelatin to the homemade dental paste causes changes in the intensity of absorption (A) of Amides I, Amides II and Amides III. The intensity increases with increasing concentration of gelatin. Therefore, ATR-FTIR is convenient in detecting the presence of gelatin in the dental materials at various concentrations.

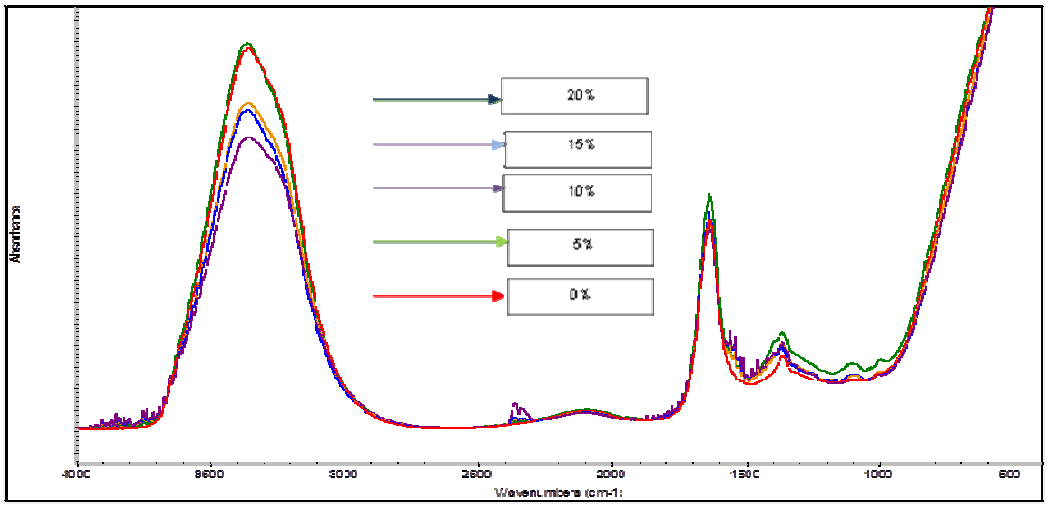


Fig 2a. Infrared spectra of homemade dental paste with added gelatin at concentration of 5, 10, 15 and 20% within a range of 4000–570. cm $^{-1}$

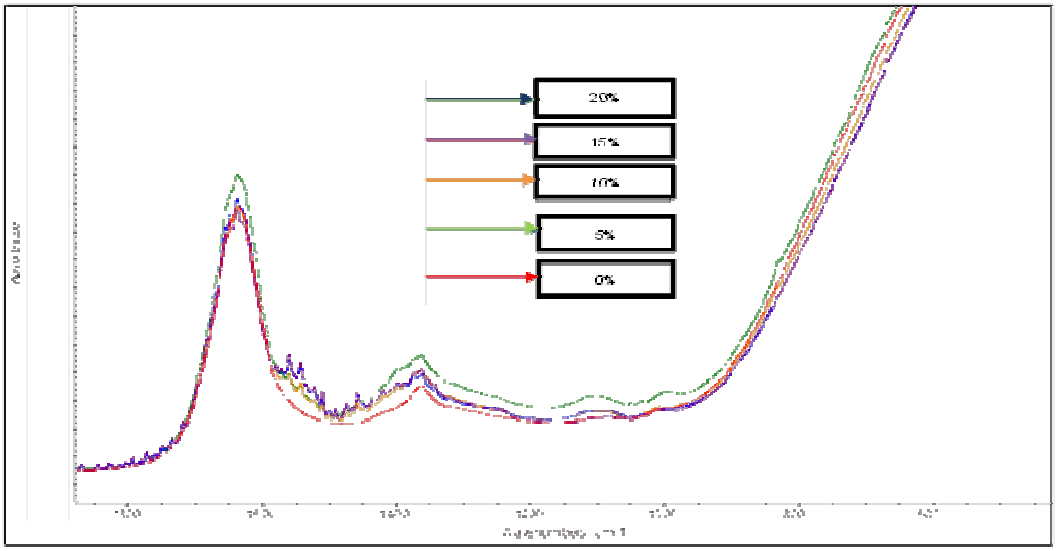


Fig 2b. Infrared spectra of homemade dental paste with added gelatin at concentration of 5, 10, 15 and 20% in the fingerprint region (1800 – 570 cm^{-1})

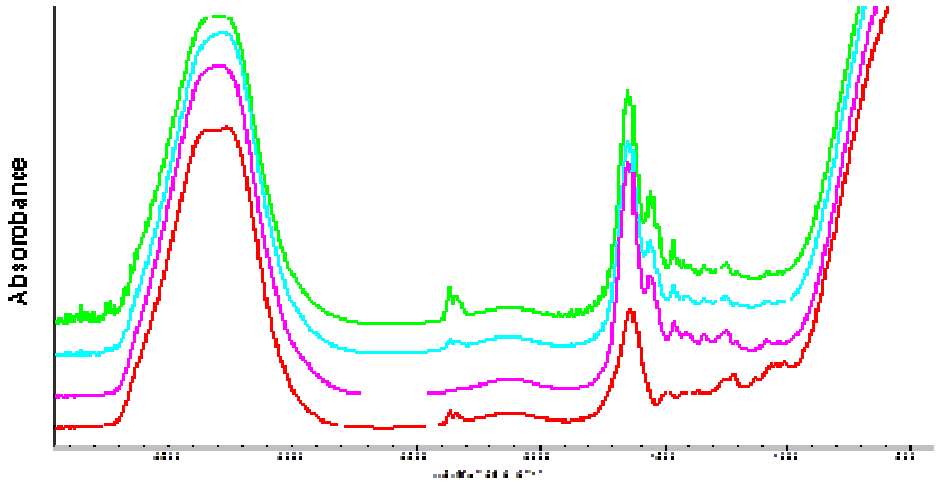
3.1.4. Detection of Gelatin In The Dental Material Samples using ATR-FTIR.

The results of gelatin detection in dental material samples are shown in Table 2, Figures 3 and 4. Comparing the spectra of the samples, the standard gelatin, and the FTIR data library in OMNIC Software, we detected 4 out of 49 samples of dental materials containing gelatin. (Figures 3 and 4; and Appendix 1, 2, 3 and 4).

Table 2. The presence of gelatin in the dental material samples

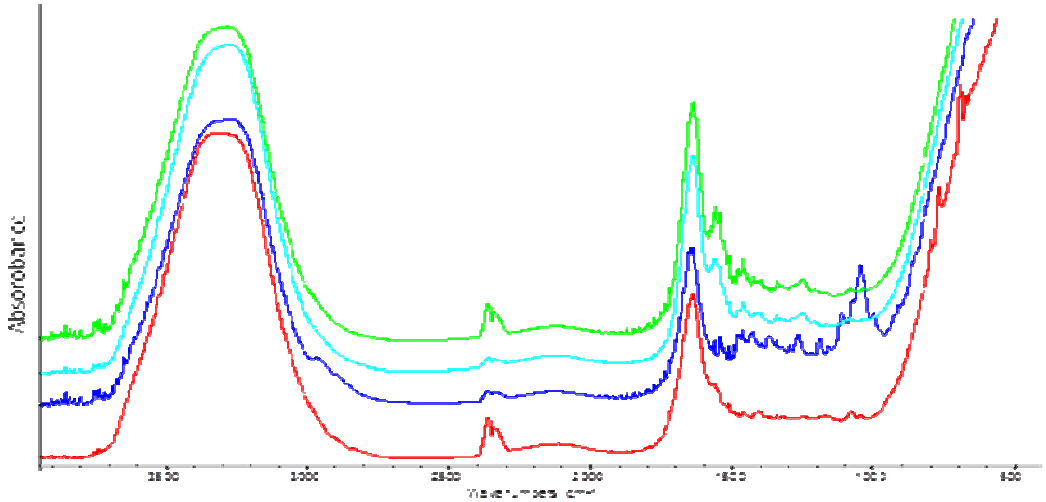
Code	Ingredient Category *	Gelatin **	Code	Ingredient Category *	Gelatin **
DM 1	P	⊕	DM 26	P	-
DM 2	I	-	DM 27	P	⊕
DM 3	I	-	DM 28	P	-
DM 4	R	-	DM 29	R	-
DM 5	I	-	DM 30	H	-
DM 6	H	⊕	DM 31	P	-
DM 7	I	-	DM 32	P	-
DM 8	I	-	DM 33	R	-
DM 9	R	-	DM 34	R	-
DM 10	R	-	DM 35	R	-
DM 11	R	-	DM 36	P	-
DM 12	P	-	DM 37	P	-
DM 13	P	-	DM 38	P	-
DM 14	P	-	DM 39	P	-
DM 15	R	-	DM 40	R	-
DM 16	R	-	DM 41	R	-
DM 17	R	-	DM 42	R	-
DM 18	P	⊕	DM 43	P	-
DM 19	R	-	DM 44	H	-
DM 20	R	-	DM 45	R	-
DM 21	R	-	DM 46	R	-
DM 22	R	-	DM 47	R	-
DM 23	R	-	DM 48	I	-
DM 24	P	-	DM 49	P	-
DM 25	P	-			

Note :
* : P = Preventive Materials
I = Impression Materials
R = Restorative Materials
H = Haemostatic Agent
** ⊕ Gelatin detected
\- No gelatin detected



Note : Green = Porcine gelatin 20% ; Violet = sample DM 6, Pale Blue = Bovine gelatin 20%; Red = Sample DM 1

Fig 3. Comparison of infrared spectra of dental materials (DM 6 and DM 1) and infrared spectra of standard bovine and porcine gelatin.



Note : Green = Porcine gelatin 20% ; Violet = sample DM 18 Pale Blue = Bovine gelatin 20%; Red = Sample DM 27

Fig 4. Comparison of infrared spectra of dental materials (DM 18 and DM 27) and infrared spectra of standard bovine and porcine gelatin

Figures 3 and 4 show the spectra of dental material samples (DM 1, DM 6, DM 18, and DM 27) compared with the spectra of standard bovine and porcine gelatin within the range of 3700-3100 cm^{-1} and 1700-1600 cm^{-1}. The spectra of these sample showed similar patterns with the standard gelatin. Therefore, it can be inferred that these four samples (DM 1, DM 6, DM 18, and DM 27) contain gelatin.

3.2. Discussion

Based on our study, the IR spectra of standard bovine and porcine gelatin showed similar patterns. Both spectra indicated 4 similar regions within the ranges 3700-2400 cm^{-1} (Amide A); 1700-1654 cm^{-1} (Amide I); 1600-1500 cm^{-1} (Amide II) and 1500-570 cm^{-1} (Amide III) (Figure 1). These results were slightly different from Irfanita et al. (2017), which might stem from the differences of resolution and the number of scan. Our study applied 4 cm^{-1} resolution and 32 scans, whereas Irfanita et al (2017) utilised 2 cm^{-1} resolution and 16 scans.

Generally, porcine and bovine gelatin showed peaks at nearly identical wavenumbers (Figure 1). However, when compared in more detailed fashion, the absorption peaks produced at each wavenumber were qualitatively different. For example, the absorbance of porcine gelatin in the Amide A region was relatively higher when compared to the absorbance of bovine gelatin, but in the Amide I and II regions (1700-1654 cm^{-1} and 1600-1500 cm^{-1}) the absorption peaks of porcine gelatin were lower than those of bovine gelatin. In addition, there were 2 peaks of amide absorption in the Amide II region of porcine gelatin, compared with 1 peak of amide absorption for bovine gelatin (Figure 1).

Absorbance within the region of 3290-3280 cm^{-1} is related to the N-H stretching and intramolecular hydrogen bond of amino acids that constitute the gelatin. Parallel polarized absorption of N-H bonds showed the interaction of hydrogen bonds in the alpha-helical structure in the gelatin structure. The resulting peak could shift to a lower frequency when the strength of hydrogen bonds in the gelatin structure increases (Hashim et al, 2010).

The double bond stretching in the C = O carbonyl group interacts with the N-H group of the peptide (C-N) bond, which appeared in the region of 1700-1654 cm^{-1}, known as the Amide I region, or as a beta-sheet structure.

The frequency in the Amide II region (1600-1500 cm^{-1}) showed the deformation of the NH group of the alphahelical structure (1550-1540 cm^{-1}) and the beta-sheet structure (1525-1200 cm^{-1}) within the polypeptide chain (Fischer et al. 2005).

According to the results of the study, it can be concluded that ATR-FTIR could be used to identify the presence of gelatin. However, this method could not be used to distinguish the origin of gelatin (whether from porcine or bovine origin). According to Jaswir (2010), FTIR method in combination with multivariate statistical analysis (chemometrics) can be used to differentiate the gelatin source from pigs and cows.

In this study, we combined the IR data with Chemometrics through Pricipal Component Analysis (PCA) and subsequent Soft Independent Modeling of Class Anology (SIMCA) tekniques in order too auteticate the gelatin source. (Branden and Hubert. 2005)

The best grouping patterns in standard porcine and bovine gelatin (at various concentrations) with normalized data within 570-1662 cm^{-1} were shown in Figures 5 and 6.

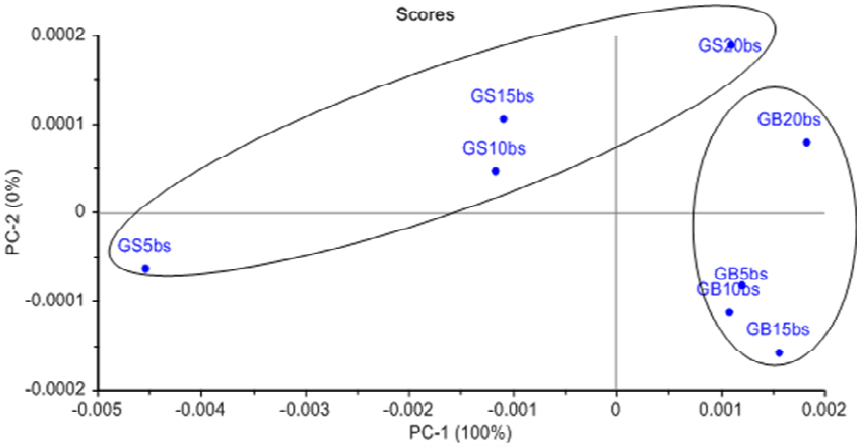


Fig 5. PCA patterns of normalised spectra of porcine and bovine gelatin at various concentration within 570 – 1662 cm^{-1}

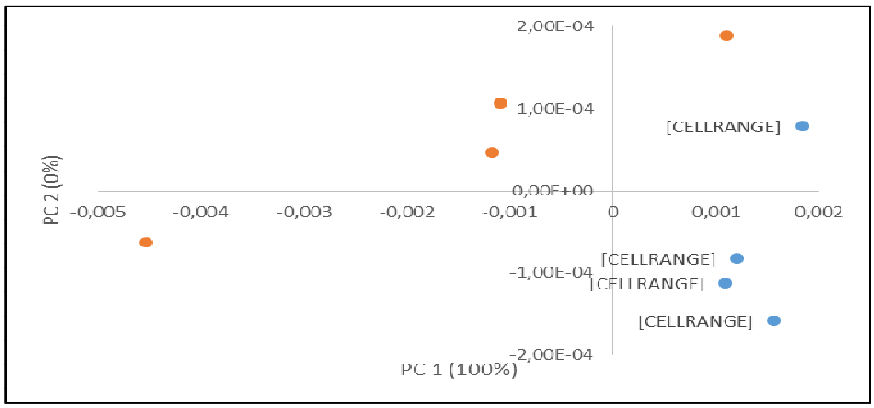


Fig 6. Score plot of PCA results of porcine and bovine gelatin at various concentrations

The initial two main components of score plot (Figure 6) were able to explain 100% of the total variance (PC-1=100%, PC-2=0%). Figure 5 shows that the grouping pattern of standard gelatin using PCA could distinguish porcine gelatin from bovine origin, except at 20% concentration. Bovine gelatin at 20% concentration could not be distinguished from porcine gelatin at the same concentration.

Further analysis was made on the dental material samples. The spectra for these samples can be seen in Figures 3 and 4. The DM18 spectra had a higher absorption than the standard gelatin spectra in the Amide III region. However, the DM18 spectra was similar to the sample spectra of Irfanita et al (2017), namely BDM 05, BDM 14, BDM 16 and BDM 31 (Appendix 5). This was due to the Si-O vibrations from the Silica hydrate compound in the DM18 which usually appear within

1200 - 800 cm^{-1} with high absorption. Based on data from OMNIC software, gelatin was detected in DM1 (with the category of Preventive material), DM6 (with the category of Haemostatic agent), DM18 (with the category of Preventive material), and DM27 (with the category of Preventive material) (Appendix 1, 2, 3, and 4).

The DM1 sample, which is in a gel form, contains water and *Chamomille recuirita* flower extract. This extract contains secondary metabolite compound (terpenoid) that is water insoluble. Therefore, in order to form a homogeneous gel mass, it needs the addition of emulsifying agents, such as gelatin. Moreover, DM1 sample also contains essential oils of *Mentha viridis* (Spearmint oil), also a water insoluble compound. Therefore, gelatin is needed to form a homogeneous gel mass.

The DM6 listed gelatin as an active (main ingredient) in its package. The spectra of DM6 looks similar with the spectra of standard porcine gelatin. The alleged presence of gelatin in the DM18 sample was related to the active ingredient of the sample, which is an anti-microbial compound (Metronidazole) in the reduced form. Therefore, in order for the ingredient to remain active, a stabilizer (like gelatin) must be added. The presence of gelatin in DM27 samples due to the addition of marshmallow as an excipient. This material contains gelatin.

The application of the PCA plot above (Figures 5 and 6), followed by SIMCA for the authentication of gelatin source in samples DM1, DM6, DM18, and DM27 were shown in Figure 7.

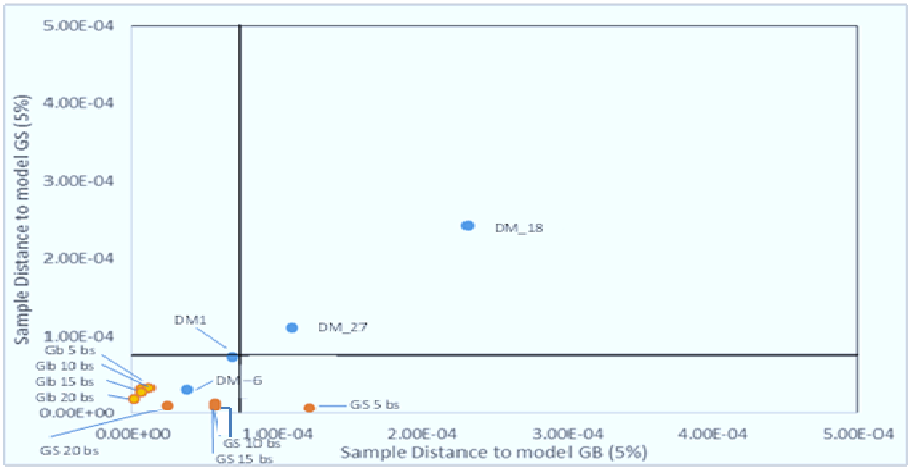


Fig 7. SIMCA result for samples DM1, DM6, DM18, and DM27
Note : Blue : Samples Yellow : porcine gelatin Orange : bovine gelatin

Figure 7 showed the clustering plot for bovine gelatin (GS, yellow) and porcine gelatin (GB, orange). This plot showed orthogonal distance from new object to the two different class (model) in the same time

Membership limit. Membership limits reflected the level of significance used in the classification. The X-axis was the model for the GB sample and the Y-axis was the model for the GS sample with a significance level for the sample influence at 5%.

According to the plot, the DM1, DM18, and DM27 data were scattered in a curve away from the grouping pattern with GB and GS. It was suspected that the concentration of gelatin in the DM1, DM18, and DM27 samples was less than 5%. It could be attributed to the factor that the gelatin was added as a emulsifying or stabilizing agent, which is usually added in the product manufacturing with a level of less than 5%. Based on the above discussion, DM1, DM6, DM18, and DM27 samples contained gelatin which functions as a raw material (for DM6 samples) and as a stabilizer or emulsifier (DM1, DM18, and DM27). The source of gelatin origin for DM6 samples was

suspected from pigs. However, the origin of gelatin for DM1, DM18, and DM27 samples could not be concluded.

4. Conclusion

The ATR-FTIR technique can be used to identify the presence of gelatin in dental materials products. Four of forty-nine dental materials used in the dental hospitals and dental clinics contain gelatin. One of them tends to be similar to pork gelatin. The other three samples cannot be deducted. Because it is suspected that the gelatin in these products serves as a stabilizer or emulsifier, which is added with a small quantity (level).

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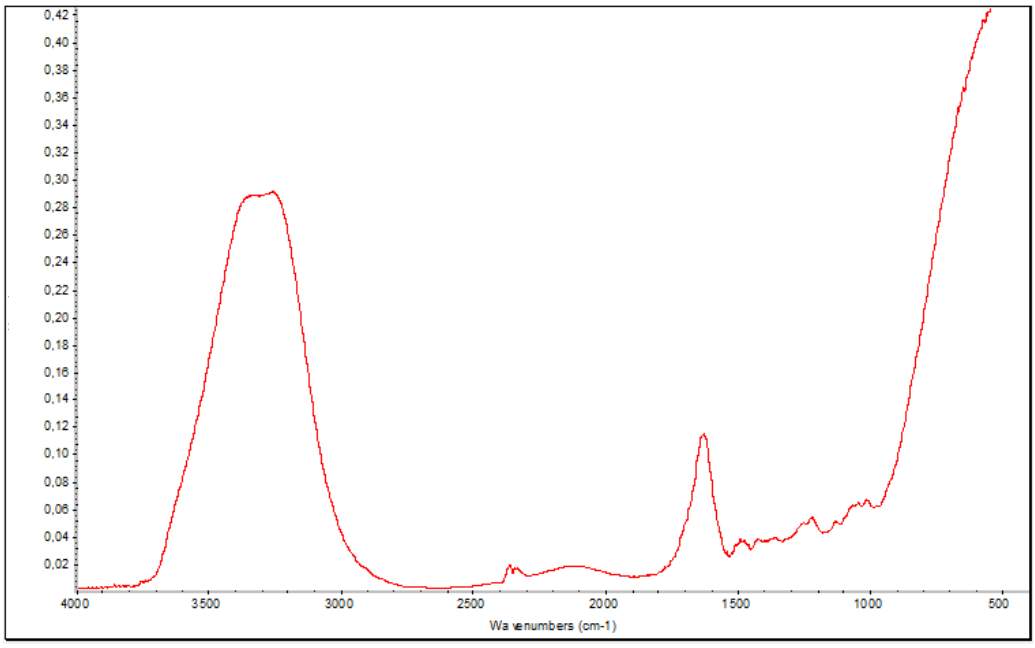
Appendix 1. Infrared Spectra of DM 1

Mon Apr 08 08:40:56 2019 (GMT+07:00)
SEARCH:
Spectrum: DM-1
Region: 3495,26-455,13
Search type: Correlation
Hit List:

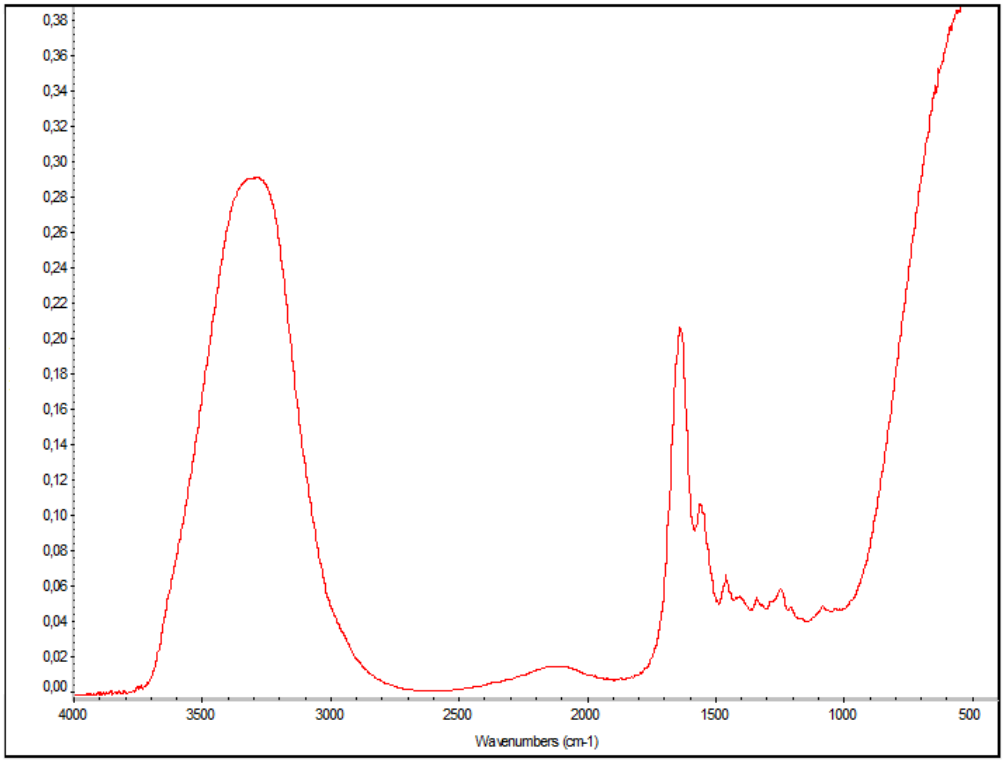
Index	Match	Compound name	Library
297	61,31	Water, Purified	HR Pharmaceutical Excipients IR Library
705	41,51	N-(2-ETHOXYPHENYL)-N-(2-ETHYLPHENYL)-ETHANEDIAMIDE	HR Nicolet Sampler Library
19	37,77	LSD TARTRATE IN KBR	Georgia State Crime Lab Sample Library
109	37,30	Gelatin	HR Pharmaceutical Excipients IR Library
290	34,76	Formaldehyde - aqueous solution	HR Nicolet Sampler Library
113	34,19	OPIUM POWDER IN KBR	Georgia State Crime Lab Sample Library
13	32,99	D-2-BROMO-LSD IN KBR	Georgia State Crime Lab Sample Library
286	31,17	Titanium Dioxide	HR Pharmaceutical Excipients IR Library
19	30,01	Lysergic acid diethylamide tartrate; LSD tartrate	HR Nicolet Sampler Library
5	29,85	LYSERGIC ACID DIETHYLAMIDE (LSD)	Georgia State Crime Lab Sample Library



Appendix 2. Infrared Spectra of DM 6

Mon Apr 08 08:45:10 2019 (GMT+07:00)
SEARCH:
Spectrum: DM-6
Region: 3495,26-455,13
Search type: Correlation
Hit List:

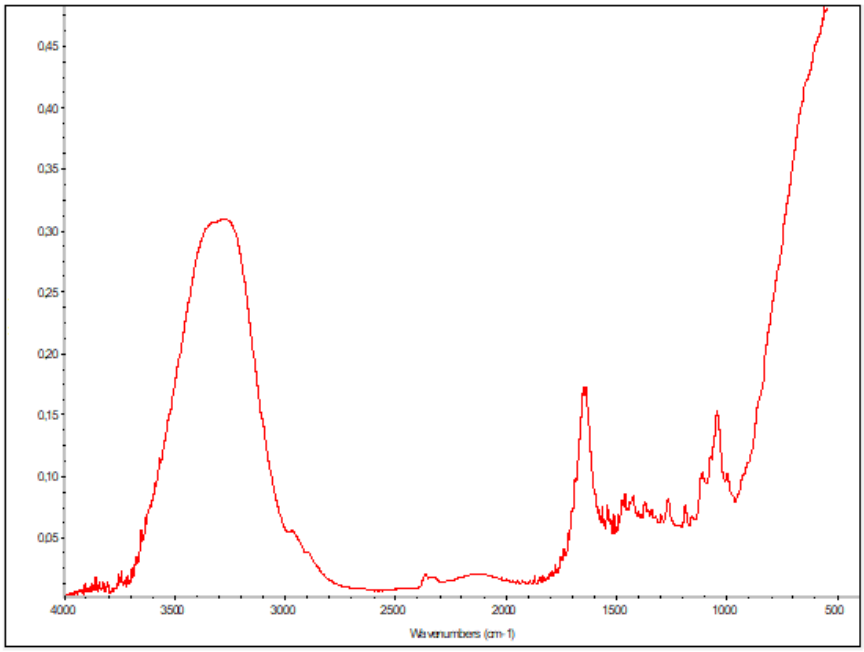
Index	Match	Compound name	Library
297	73,03	Water, Purified	HR Pharmaceutical Excipients IR Library
109	70,37	Gelatin	HR Pharmaceutical Excipients IR Library
369	49,63	D-Pantothenyl alcohol	HR Nicolet Sampler Library
705	49,04	N-(2-ETHOXYPHENYL)-N-(2-ETHYLPHENYL)-ETHANEDIAMIDE	HR Nicolet Sampler Library
19	47,70	LSD TARTRATE IN KBR	Georgia State Crime Lab Sample Library
28	45,46	POLYAMIDE 6 + POLYAMIDE 6,6	Hummel Polymer Sample Library
290	45,06	Formaldehyde - aqueous solution	HR Nicolet Sampler Library
19	44,33	BUTYRAMIDE	Aldrich Condensed Phase Sample Library
773	41,38	Polymer of phthalamide	HR Nicolet Sampler Library
1	40,50	POLYAMIDE 6	Hummel Polymer Sample Library



Appendix 3. Infrared Spectra of DM 18

Mon Apr 08 08:47:35 2019 (GMT+07:00)
SEARCH:
Spectrum: DM-18
Region: 3495,26-455,13
Search type: Correlation
Hit List:

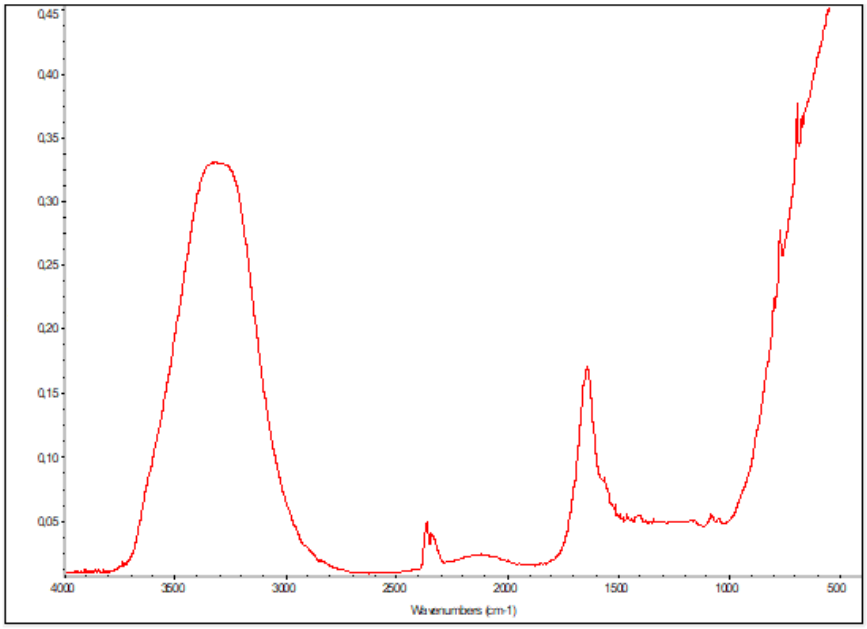
Index	Match	Compound name	Library
297	50,91	Water, Purified	HR Pharmaceutical Excipients IR Library
112	45,61	Glycerin	HR Pharmaceutical Excipients IR Library
290	44,22	Formaldehyde - aqueous solution	HR Nicolet Sampler Library
181	42,06	Monoammonium Glycyrrhizinate, 110	HR Pharmaceutical Excipients IR Library
19	41,56	BUTYRAMIDE	Aldrich Condensed Phase Sample Library
705	40,11	N-(2-ETHOXYPHENYL)-N-(2-ETHYLPHENYL)-ETHANEDIAMIDE	HR Nicolet Sampler Library
369	39,70	D-Pantothenyl alcohol	HR Nicolet Sampler Library
109	39,30	Gelatin	HR Pharmaceutical Excipients IR Library
164	39,22	Glycerol; 1,2,3-Propanetriol; Glycerine	HR Food Additives
335	38,97	Glycerol	HR Nicolet Sampler Library



Appendix 4. Infrared Spectra of DM 27

Mon Apr 08 08:46:10 2019 (GMT+07:00)
SEARCH:
Spectrum: DM-27
Region: 3495,26-455,13
Search type: Correlation
Hit List:

Index	Match	Compound name	Library
297	54,42	Water, Purified	HR Pharmaceutical Excipients IR Library
109	44,36	Gelatin	HR Pharmaceutical Excipients IR Library
705	37,37	N-(2-ETHOXYPHENYL)-N-(2-ETHYLPHENYL)-ETHANEDIAMIDE	HR Nicolet Sampler Library
181	33,57	PHENFORMIN HCL IN KBR	Georgia State Crime Lab Sample Library
19	32,69	BUTYRAMIDE	Aldrich Condensed Phase Sample Library
113	32,43	OPIUM POWDER IN KBR	Georgia State Crime Lab Sample Library
19	31,94	LSD TARTRATE IN KBR	Georgia State Crime Lab Sample Library
290	29,99	Formaldehyde - aqueous solution	HR Nicolet Sampler Library
70	28,94	PHORONE, TECH., 93%	Aldrich Vapor Phase Sample Library
369	28,21	D-Pantothenyl alcohol	HR Nicolet Sampler Library



Appendix 5. Infrared Spectra of / dental materials (Irfanita, et al. 2017)