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Debate entre a Vida Moderna e o Meio Ambiente

Cleiseano Emanuel da Silva Paniagua
(Organizador)

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APRESENTAÇÃO

O E-book: “Química: Discutindo a Vida Moderna e o Meio Ambiente” em seu volume I é composto por dezoito trabalhos científicos em forma de capítulos que buscam apresentar e promover a discussão em relação à busca por alternativas e soluções que visem ampliar o aproveitamento de matéria-prima de origem vegetal que são tratados como resíduos e até passivos ambientais. Neste sentido, a incorporação de materiais lignocelulósicos (rico em fibras, vitaminas e outros nutrientes) como matéria-prima na composição de outros alimentos vem sendo cada vez mais investigado e aplicado tanto na nutrição animal quanto na humana. Além disso, a biomassa vegetal vem sendo estudada para: (*i*) produção de materiais e utensílios com propriedades semelhantes às encontradas em matérias-primas virgens provenientes de fontes não renováveis e que causam grandes impactos ao ambiente tanto em sua extração quanto no descarte após sua utilização; (*ii*) produção de combustíveis oriundos de fontes renováveis e que causam menor impacto ao meio ambiente; (*iii*) materiais com alta capacidade de remoção de poluentes presentes em diferentes matrizes aquosas e com enorme potencial para serem utilizados tanto em substituição quanto na complementação de etapas convencionais de tratamento de água e esgoto.

Neste contexto a busca por novos materiais; tecnologias que proporcionam maior rapidez, menor consomem de reagentes, reaproveitamento de materiais, solventes menos tóxicos e produzidos a partir de fontes renováveis vêm ganhando cada vez mais espaço e se constituindo na chamada Química Verde.

No entanto, apesar de todos os esforços que vem sendo feitos nos diferentes setores da industria, pesquisa e tecnologia na busca por processos ecologicamente mais corretos e sustentáveis, o estilo de vida da população fundamentado no consumo além da necessidade vem ocasionando inúmeros impactos ambientais tanto a biota aquática quanto aos diferentes ecossistemas do planeta Terra, tendo nos recursos hídricos o principal meio de propagação de substâncias provenientes de inúmeras fontes, em especial pelo sistema de saneamento básico e pela aplicação de pesticidas nas atividades agropecuárias.

Neste contexto, inúmeras técnicas de detecção e quantificação em escala traço (ng a μg L^{-1}) vem se destacando pela miniaturização ou capacidade de detectar e quantificar inúmeras classes de compostos (resíduos de fármacos, pesticidas, drogas ilícitas, hormônios, dentre outros) que se constituem em uma classe de substâncias na qual não se conhece os possíveis efeitos deletérios a médio e longo prazo para a saúde humana e do ambiente.

Com o intuito de colaborar tanto na divulgação quanto na disseminação de novos conhecimentos, a Atena Editora organiza e publica trabalhos de alta relevância, disponibilizando de forma gratuita em diferentes plataformas de busca e pesquisa.

Cleiseano Emanuel da Silva Paniagua

SUMÁRIO

CAPÍTULO 16

A STATISTICAL MULTIVARIATE APPROACH TO EVALUATE FLUORINE CONTENT IN BRAZILIAN TOOTHPASTES

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ABSTRACT: This work investigated the similarity between chemical compositions described in the packaging of Brazilian toothpaste samples and the concentrations of total available fluorine, free fluorine, and pH were determined. Both HCA and PCA were used to evaluate the similarities in chemical compositions and sample distinctions. All 41 samples were assigned into 5 groups in HCA. In samples with Na_2PO_3F and $CaCO_3$ used as fluorine source and abrasive, respectively, the average of total available fluorine concentration relative to the fluoride value described in the packages was 40.2%, which was lower than the 74.7% found in toothpastes with NaF and silica. pH values ranged from 5.82 to 9.53. The PCA showed that the formulations based on NaF and silica presented higher concentrations of free fluoride. It can still be inferred that samples with higher free fluorine concentrations have the lowest pH values.

KEYWORDS: Toothpaste, Available fluorine, Multivariate analysis.

UMA ABORDAGEM ESTATÍSTICA MULTIVARIADA PARA AVALIAR O FLÚOR CONTIDO EM DENTIFRÍCIOS BRASILEIROS

RESUMO: Este trabalho investigou a semelhança entre as composições químicas descritas nas embalagens de dentifrícios brasileiros e foram determinadas as concentrações de flúor total disponível, flúor livre e pH. HCA e PCA foram usados para avaliar as semelhanças nas composições químicas e distinções das amostras. Todas as 41 amostras foram divididas em 5 grupos em HCA. Em amostras com Na_2PO_3F e $CaCO_3$ utilizadas como fonte de flúor e abrasivo, respectivamente, a média da concentração total disponível de flúor em relação ao valor de flúor

descrito nas embalagens foi de 40,2%, que foi inferior aos 74,7% encontrados em pastas de dente com NaF e sílica. Os valores de pH variaram de 5,82 a 9,53. O PCA mostrou que as formulações baseadas em NaF e sílica apresentaram maiores concentrações de flúor livre. Ainda pode ser inferido que as amostras com maiores concentrações de flúor livre têm os menores valores de pH.
PALAVRAS-CHAVE: Dentifrícios, Flúor disponível, Análise Multivariada.

1 | INTRODUCTION

Fluorides are found in the human body in small quantities (3 mg in adults), on average. However, they are beneficial in preventing tooth decay when ingested at the concentration of 0.05 mg.kg^{-1}of body weight per day (RETO et al., 2008). Fluorine strengthens and favor remineralization of tooth enamel and dentin, not only because they reduce the solubility of these compounds in acid medium, but also because they reduce the bacterial capacity to produce acids (FERNÁNDEZ; TENUTA and CURY, 2016).

The use of fluoride-containing (F^-) dentifrices has been identified as one of the factors responsible for the decrease in dental caries in the last decades (CURY, 1987). The act of brushing promotes disorganization of the dental biofilm (dental plaque) while the concentration of fluoride is increased in the oral cavity. However, this fluoride should be chemically compatible with the formulation of the toothpaste to ensure anticaries effectiveness (CURY and TENUTA, 2008).

Fluoride in its free ionic form (F^- from sodium fluoride, NaF) or its ionizable form (sodium monofluorophosphate, Na_2PO_3F) ensures its bioavailability and abundance in the mouth and the anticaries activity (TEN CATE and FEATHERSTONE, 1991). Also, many studies have concluded that dentifrice formulations should contain a concentration of at least 1,000 ppm of fluorine to present the anticaries effect (MARINHO; HIGGINS and LOGAN, 2003). To have a high bioavailability, the chemical source of F and the abrasive mustn't interact.

Toothpastes have several components in their composition, so many interactions occur in their formulations. Multivariate data analysis, mainly principal component analysis (PCA) and hierarchical cluster analysis (HCA), allow the evaluation of the relationship of multiple variables together. The use of HCA allows for the evaluation of similar groupings according to the components present or absent in the formulation of toothpastes of different brands and to associate to the manufacturer's information. Through the PCA it is possible to identify the existing interactions by the loadings of the principal components (PC), being able to define the best conditions for the interaction of the source of fluoride and the abrasive component to be decreased, i.e., to define the best formulation parameters to increase the anticaries potential

Considering the effectiveness of fluoride toothpastes, the objective of this study was to compare the amounts of total available F^-, free or ionic F^-, and pH to the total amounts

described in the packages of samples of toothpaste sold in Brazil. Besides, this study aimed to analyze the similarity of the chemical compositions between these samples.

2 | EXPERIMENTAL

2.1 Samples

Dentifrice samples of different brands containing fluorine were randomly acquired in Santa Maria, RS, Brazil. The samples included dentifrice for children and adults, totalizing 41 samples. After the acquisition, the products were stored at room temperature and kept properly closed to avoid any alteration of the samples.

2.2 Information from the packaging

All samples were checked for information on the package, either in the outer carton or in the tube itself. The source of fluorine and its concentration in parts per million (ppm), the abrasives used in the composition and the pharmacotechnical form (gel or cream), were taken directly from data provided by the manufacturers. The expiration date for each sample was also observed to ensure that all of them were analyzed within shelf life. The expiration date for each sample was also observed to ensure that all of them were analyzed within shelf life.

2.3 pH measurements

For pH measurements, the samples were prepared according to ISO 11609:2010. After opening the tube, the first 5 grams of sample to be removed were discarded. Then, 10 g of toothpaste was added to 30 mL of deionized water and stirred till a homogenous suspension was obtained. After 3 minutes, pH was analyzed in a pH meter (MS Tecnopon™) with temperature control at 25± 0.1 ºC. All measurements were performed in triplicate.

2.4 Measurements of Total Available Fluorine and Free Fluorine

The concentrations of fluorine in toothpaste were determined according to a protocol described by several studies (CURY et al., 1981; DELBEM, VIEIRA and CURY, 2002; CURY et al., 2010; RICOMINI et al., 2012; SEBASTIAN and SIDDANNA, 2015). All measurements were performed in triplicate.

The samples were prepared in two different ways, according to the form of fluorine to be measured. For determination of free F^-, the dentifrice samples were weighed (0.500 g), dissolved in deionized water under stirring for 2-5 minutes, and sonicated for another 10 minutes. Then, 1 mL of TISAB III buffer solution (1.0 mol L^{-1} acetate buffer, pH 5.0, containing 1.0 mol L^{-1} NaCl and 0.4% CDTA (acid cyclohexanediamine tetraacetic) was added, and the solution was made up to the mark of 50 mL with deionized water. For the determination of total available F^-, 0.5 g the dentifrice samples were dissolved in deionized water under stirring for 2-5 minutes and sonicated for another 10 minutes. Then, 2 mL of 2

mol L^{-1} HCl (Vetec) was added to the suspensions. They were kept under heating (45 ºC) and stirred for 60 minutes. After cooling, the solutions were neutralized with 1 mol L^{-1} NaOH (Êxodo Científica). Finally, 1 mL of the TISAB III buffer solution was added and the solution was made up to the mark of 50 mL with deionized water.

The determinations of free and total fluoride content were performed by potentiometry using a fluoride ion-selective electrode (Thermo, model Orion 96-09). The solutions were stirred during all measurements and a Table reading of the electrode potential was achieved after 3 minutes.

The analytical curve was constructed with concentrations of 0.5, 1.0, 5.0, 10.0, 20.0, and 50.0 ppm of F^-, from a stock solution of 1000 ppm of F^-. Then, electrode potential (mV) measurements *versus* logarithm of concentration were plotted, which were accepted when $r^2 \geq 0.99$. For every ten readings, a new calibration was performed.

2.5 Statistical Multivariate Analysis

The results are presented as mean and standard deviation of the mean. The statistical multivariate methods used for comparison and synthesis or simplification of the results were HCA and PCA.

For the clustering analysis, the total composition of each sample was used, i.e., all components were tabulated as variables, where their absence was represented by the number zero and their presence by the number one, which resulted in 41 rows (toothpaste samples) and 67 columns (information variables). The Euclidean distance was used as a measure of dissimilarity, and the dendrogram was constructed using the method of complete linkage (furthest neighbor). Statistical multivariate analysis was performed using the software R_{Studio} (version 3.3.3).

The results obtained for total fluoride concentration, free fluoride, pH, as well as qualitative variables such as fluorine source, pharmacotechnical presentation, abrasives, and target audience were analyzed and evaluated through PCA using the correlation matrix. Statistical multivariate analysis was performed using the software R_{Studio} (version 3.3.3).

3 | RESULTS AND DISCUSSION

3.1 Information from the packaging and Hierarchical Cluster Analysis

A frequency survey of all the components described in the packages of the 41 studied samples was performed (Figure 1). Also, research on the function of each of these components within the toothpaste was carried out.

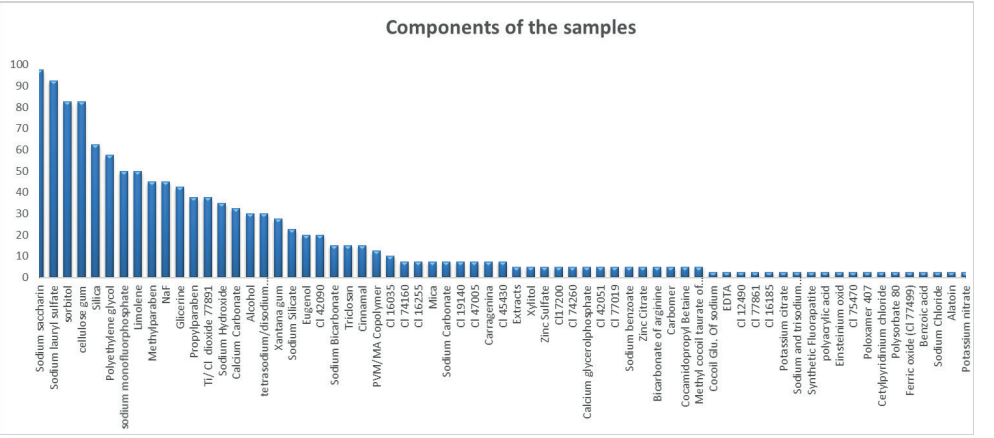

Figure 1. Frequencies of the components described in the packaging of the 41 analyzed dentifrices.

Components that are present in the majority of the samples are shown in larger columns. For example, components such as sodium saccharin, which is a sweetener responsible for leaving toothpaste with a sweet taste (MARTINS et al., 2012), is present in 100% of the samples.

Each component has a function to ensure the cosmetic and preventive or therapeutic effects of the formulation, such as the abrasives, which are responsible for the mechanical cleaning of the teeth and for controlling the accumulation of stains therein. Substances with preventive or therapeutic functions, like fluoride salts, are also of great importance (CURY, 1987). Among the studied dentifrices, two abrasives are commonly present: silica dioxide (SiO_2) and calcium carbonate ($CaCO_3$). Two sources of fluorine were present: NaF, present in 46.3% of the toothpaste, and Na_2PO_3F, present in 48.8% of the samples.

HCA analysis was performed to analyze the similarities between the compositions of the samples. In the dendrogram shown in Figure 2, it is possible to observe the grouping for each sample. Euclidean distance was used, which was measured by the presence or absence of the components in the samples. The dendrogram was constructed from a distance matrix for each element, in which the vertical scale indicates the level of similarity (or dissimilarity), and the samples are arranged perpendicular to the dimensional axis.

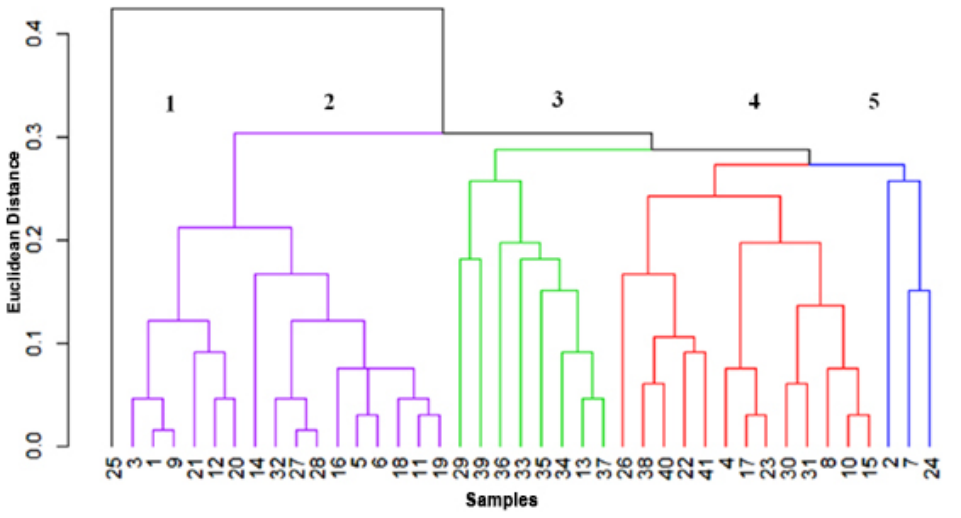

Figure 2. Dendrogram obtained by HCA using all the components described on the sample packages.

The dendrogram shows a maximum distance of 0.4, that is, in this distance, there is only one group that is represented by all the samples. Below the distance 0.3, it may be observed a heterogeneous separation of 5 groups, each one formed by its samples with greater similarity in composition. This division into 5 distinct groups is due to the complexity in the composition of each sample. Manufacturers, driven by consumer demand in recent decades, have introduced several other purposes to tooth brushing, such as bleaching, gingivitis prevention, erosion and/or dental hypersensitivity, refreshing flavors (LIPPERT, 2013). Toothpastes intended to reduce sensitivity, for example, usually, present components beyond those in a toothpaste intended only for caries prevention This optimization of formulations increases their complexity and may affect the availability of fluoride in toothpaste (SJÖGREN, 2001).

The first group is formed only by sample 25. This toothpaste presented 25 components in its packaging while the average found for the other samples was 15 components, which made it different from the others.

The second group is characterized by containing the largest amount of dentifrice samples (3,1,9,21,12,20,14,32,27,28,16,5,6,18,11 and 19). The samples are grouped by their similarity in terms of fluorine source and abrasive component. Except for sample 14, which has source of fluorine the NaF and do not have abrasive, all samples have Na_2PO_3F and $CaCO_3$ as source of fluorine and abrasive, respectively. In the third group, samples 37, 13, 34, 35, 33, 36, 39 and 29 are grouped. This group was formed by all the samples having SiO_2 as abrasive component.

The fourth group is formed by samples 26, 38, 40, 22, 41, 4, 17, 23, 30, 31, 8, 10 and 15. All samples in this group have NaF and SiO_2 as source of fluorine and abrasive, respectively. In the fifth and last group, there are only 3 samples (2, 7 and 24), the three samples are dentifrices to reduce the sensitivity and regeneration of tooth enamel, having its composition other substances for these functions, differentiating from the others.

3.2 Measurements of total fluoride, free fluoride, pH and Components principal analysis

The concentrations of total available F^- and free F^- present in the samples were determined based on the equations of the analytical curves (Tables 1 and 2) obtained from external calibration.

Calibration curve equation	r^2	Samples
y= -34.45x + 1.89	0.995	17/5/11/3/6/Spike (17 and 6)*
y= -33.57x + 4.44	0.997	8/13/14/30/31
y= -32.18 + 5.42	0.994	37/29/39/22/23/24
y= -30.76x + 3,22	0.993	19/21/26/27/28/1
y= -30.87x + 5.98	0.996	32/33/34/38/40/41
y= -26.14 + 0.25	0.993	20/16/15/25/10
y= -29.81 + 2.00	0.993	18/9/4/12/2/7

*standard addition (10 ppm in 50 mL of sample)

Table 1: Available total F^- analytical curves

Calibration curve equation	r^2	Samples
y= -25.75x - 9.20	0.994	17/18/19/20/29/Spike (17) *
y= -27.25x -6.19	0.995	14/15/16/35/36
y= -26.30x - 15.27	0.996	10/11/12/13/28
y= -25.50x - 7.30	0.991	26/27/30/31/32/33/34
y= -24.71x - 5.49	0.996	32/33/34/38/40/41
y= -34.09x - 19.44	0.990	6/7/8/9/21/Spike (6) *
y= -47.33x - 5.13	0.998	1/2/3/4/5
y= -33.09x - 7.23	0.994	21/22/23/24/25

*standard addition (10 ppm in 50 mL of sample)

Table 2: Free F^- analytical curves

The results showed that all toothpaste analyzed in this study did not contain higher concentrations of available fluorine than those described in the packages, as shown in Table 3, all concentration values of total F^- and free F^- were below 1,500ppm, which is the

maximum value allowed by Resolution 79 (BRASIL, 2000).

Of the 41 toothpastes analyzed, only 22 presented more than 50% of the fluoride described on the packaging. In samples with Na_2PO_3F and $CaCO_3$ used as fluorine source and abrasive, respectively, the average of total available fluorine concentration relative to the fluoride value described on the packages was 40.2%, which was lower than the 74.7% found in toothpaste with NaF and silica. The free F^- concentrations varies considerably from 8.9% (sample number 10) to 93.8% (sample 9). While in total F^- the variation is smaller, from 23.6% (sample 1) to 96.0% (sample 15). Regarding pH measurements, it was observed a great variation in the results, which ranged from 5.82 (sample 39) to 9.53 (sample 29).

As described by Benzianet al. (BENZIAN et al., 2012), the literature does not yet provide conclusive information on which of the available free fluoride concentrations in toothpaste show the best anticaries efficacy. As a consequence, the Brazilian resolution and international regulations, such as the European and the one for cosmetic products in Mercosul, only specify the total fluoride and its products, which should not exceed 1,500 ppm of F (BENZIAN et al., 2012). The only exception is the US Food and Drug Administration guidelines that state that toothpaste with NaF and Na_2PO_3F containing 850-1,150 ppm of total fluorine should contain ≥ 650 ppm and ≥ 800 ppm of available fluorine, respectively (FDA, 2017; LIPPERT, 2013).

In the Brazilian, European Union (EU) and Mercosul regulations, fluoride compounds are regulated as a cosmetic, and about 20 different compounds are allowed. Mixtures of various fluorine compounds are permitted since the maximum concentration of fluorine does not exceed 1,500 ppm. It is to be noted that several of the allowed fluoride compounds (e.g., CaF_2, MgF_2) are only moderately soluble (MERCOSUL, 2017; UNITED KINGDOM, 2017). In the USA, fluoride compounds are regulated as drugs and hence fewer fluoride compounds are allowed (LIPPERT, 2013).

Thus, even following the Anvisa resolution currently in effect in Brazil, many of the studied toothpaste present low concentrations of total and available F, and even smaller quantities of free or ionic F. According to previous studies, it is a requirement that the F contained in the dentifrice is active (CURY and TENUTA, 2008; BENZIAN et al., 2012; CURY et al., 2004; CARRERA et al., 2012; NARVAI, 2006).

Samples	Samples code	F label (ppm)	Total available F^-(ppm)	Free F^-(ppm)	pH	F source		Abrasive		A/C*		Pharmacote-chnical form	
						NaF	Na_2PO_3F	Silica	$CaCO_3$	A	C	Gel	Cream
Colgate menta refrescante	1	1450	342.3± 35.0	225.6± 14.1	9.00± 0.01		X		X	X			X
Colgate sensit. Multiprot.	2	1450	909.7± 68.0	135.6± 17.3	7.68± 0.02		X	X		X			X
Colgate Neutraçúcar	3	1450	447.7± 66.2	178.3± 21.3	8.75± 0.02		X		X	X			X
Colgate T 12 gel adv. fresh	4	1450	1311.4± 61.3	993.2± 78.6	8.10± 0.03	X		X		X		X	
Alg creme dental	5	1500	609.4± 2.2	182.0± 13.6	7.82± 0.06		X		X	X			X
Alg kids –tutti frutti	6	1100	626.0± 79.6	116.7± 13.4	7.80± 0.15		X		X		X		X
Regenerate	7	1450	621.3± 23.1	502.9± 51.1	8.89± 0.03		X	X		X			X
Tandy tutti frutti	8	1100	818.1± 70.6	1032.1± 44.0	6.93± 0.10	X		X			X	X	
Sorriso dentes brancos	9	1450	408.8± 24.9	128.1± 2.2	8.89± 0.02		X		X	X			X
Tandy uva ventura	10	1100	847.8± 52.9	885.3± 85.0	6.36± 0.20	X		X			X	X	
Ice Fresh	11	1500	484.6± 86.8	144.3± 4.8	8.79± 0.05		X		X	X			X
Colgate tripla ação	12	1450	420.8± 19.3	149.5± 9.4	9.22± 0.03		X		X	X			X
Ice fresh over gel	13	1500	1417.9± 45.3	1044.3± 28.3	6.84± 0.20	X		X		X		X	
Dentplaque	14	1100	1055.6± 45.3	883.8± 88.4	6.26± 0.14	X		---	---	X		X	
Tandy morango	15	1100	692.4± 28.4	703.4± 19.6	7.10± 0.05	X		X			X	X	
Contente plus	16	1500	519.7± 9.5	177.2± 1.7	7.86± 0.10		X		X	X			X
Colgate 12 profes. clean	17	1450	871.0± 12.1	1092.5± 47.6	7.94± 0.03	X		X		X			X
Tralálá kids morango	18	1100	312.5± 19.5	165.2± 29.0	9.09± 0.06		X		X		X		X
Ice fresh brancos	19	1500	449.9 ± 40.7	162.0± 23.6	8.93± 0.05		X		X	X			X
Colgate menta original	20	1450	490.5 ± 62.1	173.8± 14.4	9.13± 0.01		X		X	X			X
Colgate pró alívio	21	1450	500.0± 20.4	150.0± 17.0	8.71± 0.20		X	X		X			X
Colgate spiderman	22	1100	791.7± 54.6	895.6± 61.8	8.20± 0.20	X		X			X	X	

Colgate T12 clean mint	23	1450	1088.2± 59.6	1312.0± 77.1	7.93± 0.02	X		X		X			X
Sensodyne Repair	24	1426	669.0± 30.6	137.1± 29.9	9.08± 0.20		X	X		X			X
Oral-B complete	25	1100	672.8± 14.9	716.7± 50.3	8.18± 0.01	X		X		X			X
Prevent Antiplaca	26	1200	553.3± 20.4	163.6± 19.3	6.53± 0.07		X	X		X			X
Ultra Action Menta	27	1200	409.0± 2.8	179.7± 18.7	8.43± 0.09		X		X	X			X
Ultra Action Hortelã	28	1200	322.6± 18.6	203.2± 32.3	8.41± 0.01		X		X	X			X
Sensodyne Branq.	29	1384	900.1± 54.6	621.4± 26.2	9.53± 0.09	X		X		X			X
Clouse up Ação profunda	30	1450	1155.9± 64.9	891.3± 3.9	7.42± 0.10	X		X		X		X	
Close up Fire + Freeze	31	1450	1004.0± 10.3	860.5± 9.8	6.74± 0.01	X		X		X		X	
Ultra Action Eucalipto	32	1200	382.4± 5.0	154.8± 17.0	8.35± 0.10		X		X	X			X
Bitufo Gel Dental	33	1450	860.6± 5.3	174.4± 19.5	6.34± 0.01		X	X		X		X	
Sanifill Gel Menta	34	1450	1128.7± 2.5	832.7± 77.9	6.94± 0.07	X		X		X		X	
Bitufo Cocoricó	35	0	Not Found	Not Found	6.68± 0.02	----	----	X			X	X	
Sanifill patati patatá	36	0	Not Found	Not Found	6.15± 0.03	----	----	X			X	X	
Boni Gel Dental Uva	37	1100	916.1± 72.3	807.8± 47.0	6.65± 0.03	X		X			X	X	
Ultra Action Kids	38	1100	659.6± 75.8	733.2± 22.6	6.65± 0.03	X		X			X	X	
Sanifill Kids Rio 2	39	1100	880.6± 15.0	846.6± 11,7	5.82± 0.03	X		X			X	X	
Boni Looney Tunes	40	1100	694.6± 83.3	855.8± 79.6	6.88± 0.20	X		X			X	X	
Gel Dental Bambinos2	41	500	313.5± 21.73	298.7± 8.7	6.59± 0.06	X		X			X	X	

* A and C stand for toothpastes intended for adults and children, respectively.

Table 3. Values found for pH, total and free fluoride, as well as packaging information presented in the labels of the 41 analyzed samples.

PCA (Figure 3) showed that the first (PC1) and second (PC2) the 57.02% and 23.55% of the total observed variance, respectively, totaling 80.1% of data variance. So, PC1 and PC2 were selected for modeling the data. The variance observed in PC1 is due to the variables NaF, silica, $CaCO_3$, gel, cream, Na_2PO_3F, pH and free F^-. Therefore, they contribute to discriminate the set of dentifrice samples in this component. On the other

hand, the variance explained by PC2 was due to the variables fluorine in the label, total F^-, adult and child.

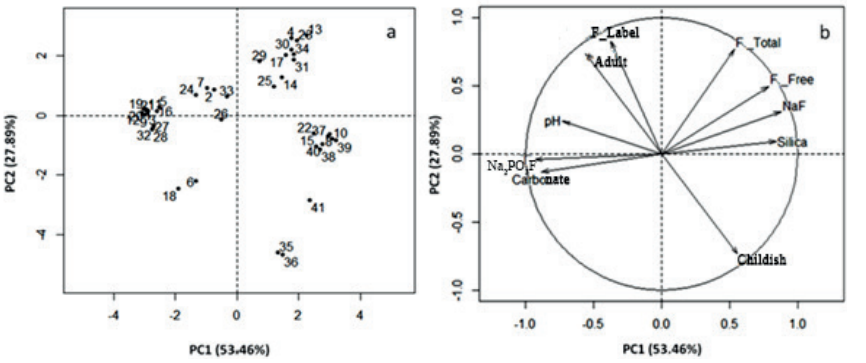

Figure 3. Scores (a) and loadings (b) plots of the distribution of 41 toothpaste samples considering the variables fluorine label, total fluorine (available), free fluorine (ionic), pH, (NaF, Na_2PO_3F), abrasive used (silica or $CaCO_3$), guidance for use (adult, children), pharmaceutical form presented (gel, cream).

Comparing Figure 3a with Figure 3b, it is possible to observe a separation of the samples along the PC1. In the negative region of this PC, we find samples that contain Na_2PO_3F as source of fluorine in their formulations, present cream as pharmacological form, $CaCO_3$ as an abrasive and present high pH values. On the other hand, in the positive region are the samples referring to the formulations of NaF as a source of fluorine, gel as pharmacotechnical form and silica used as abrasive agent. Also, in this region, we can find the samples with higher pH values, when compared to the other samples.

PCA analysis indicates that formulations based on NaF and silica have higher free F^-concentrations, since these variables are found in the negative region along PC1. That is, there is a positive correlation between them (Figure 3b). The same relationship occurs between pH, $CaCO_3$ and Na_2PO_3F as the source of fluorine.

We can still infer that the samples with the highest free F^- concentrations also had the lowest pH values. In Figure 3a, it is possible to note that the samples that are distributed along the PC1 elucidate this contrast, where the samples with lower pH and higher concentrations of F^- are located in the more negative region of PC1. Buzalaf, Ogaard and Vogel observed in their studies that there was an increase in the effectiveness of dentifrices in acid pH, due to the higher formation of CaF_2 on the dental surface (BUZALAF and LEVY, 2011; ØGAARD, 2001; VOGEL, 2011). In another study, it was demonstrated that the amount of CaF_2 formed after treatment with an acid dentifrice with low F concentration (NaF, 550 ppm of F, pH 5.5) was equivalent to that obtained after the use of a commercial dentifrice containing 1,100 ppm of F (NEGRI and CURY, 2002).

PCA analysis also showed a difference between the bioavailability of fluorine from

NaF and from Na_2PO_3F. It is not expected that the final amount of fluoride of both compounds will be different in the mouth, but the amount of ionic fluoride will be considerably lower for the toothpaste with Na_2PO_3F (BRUUN, GIVSKOV and THYLSTRUP, 1984).

Comparing mouth rinsing based on NaF and Na_2PO_3F, Vogel et al. (2000) showed that NaF promoted a higher bioavailability of fluoride in saliva and biofilm fluid when compared to Na_2PO_3F (VOGEL et al., 2000). However, little is known about the parameters involved in the hydrolysis of the Na_2PO_3F in the biofilm, such as its diffusion, the subsequent conversion to ionic fluoride, and the pH effect of the toothpaste, which may affect the phosphatase activity *in vivo* (FALCÃO, TENUTA and CURY, 2013).

One advantage of toothpaste containing Na_2PO_3F is that it can be formulated along containing abrasives with calcium because of the excellent compatibility with the monofluorophosphate ion (LIPPERT, 2013). In a study on the efficacy of fluoride use described in the WHO Bulletin, it was suggested $CaCO_3$ to be chosen as abrasive agent due to its low cost and greater availability in developing countries (JONES, 2005). However, a study describing the clinical trials admits that $CaCO_3$ is not perfectly compatible with the Na_2PO_3F because, toothpaste age they lose their available free fluoride, particularly those with formulations based on Na_2PO_3F and abrasives containing Calcium (BARDAL, 2003). In a study on the fluoride concentration in the dentifrices based on sodium monofluorophosphate and calcium carbonate, Cury observed that the fluoride concentration monitored during two years of storage at 25 ºC had an average reduction of 28% (CURY, CALDARELLI and TENUTA, 2015).

It is also possible to observe the dispersion of the two samples (35 and 36) which did not contain fluorine in their formulation. These were very distant from the other samples in the most negative region along PC2.

4 | CONCLUSIONS

- In the 41 toothpaste samples, 68 compounds were found present in its formulations being NaF and Na_2PO_3F the main sources of fluorine and $CaCO_3$ and Silica the main abrasive components.
- Using the HCA, it was possible to separate the samples into 5 similarity groups. The groups are formed mainly by the presence of pairs of fluorine sources and abrasives.
- Samples that have Na_2PO_3F and $CaCO_3$ as a source of fluorine and abrasive respectively have 34.5% less fluoride available than samples with NaF and $CaCO_3$.
- The PCA showed the difference in the bioavailability of fluoride with NaF and Na_2PO_3F, confirming that Na_2PO_3F compounds have lower availability. Thus, it is possible to confirm that statistical tools can help in the search for answers

already experimentally proven, facilitating future work.

- Although both experimental and statistical results show that Na2PO3F as a source of fluorine has lower availability of fluorine, it is still not possible to state that toothpastes with this compound are more effective in preventing caries to NaF because there is no consensus of a minimum concentration of fluorine more effective for this prevention.

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