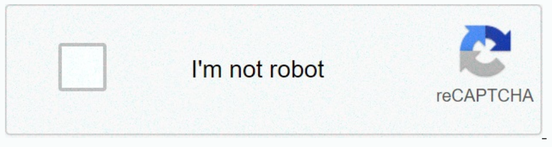

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Atr fourier transform infrared spectroscopy

An ATR accessory measures the changes that occur in an internally reflected IR beam when the beam comes into contact with a sample. An IR beam is directed to an optically dense crystal with a high refractive index at a certain angle. This inner reflection produces an evanescence wave that extends beyond the surface of the crystal into the sample held in contact with the crystal. In regions of the IR spectrum where the sample absorbs energy, the evanescence wave is attenuated. The attenuated beam returns to the crystal, then leaves the opposite end of the crystal and is directed to the detector in the IR spectrometer. The detector records the attenuated IR beam as an interferogram signal, which can then be used to generate an IR spectrum. Watch the Request Consultation ATR video series, which is ideal for highly absorbent or thick samples that often produce intense peaks when measured by transmission. ATR is well suited for these samples because the intensity of the evanescent waves decays exponentially with the distance from the surface of the ATR crystal, which makes the technique generally insensitive to sample thickness. Other solids that are well suited for ATR are homogeneous solid samples, the surface layer of a multilayer solid or the coating on a solid. Even irregularly shaped hard solids can be analyzed with a hard ATR crystal material such as diamond. Ideal solids are: Laminate colors Plastics rubber coatings Natural powder solids that can be ground in powder In addition, ATR is often the preferred method for liquid analysis because it simply needs to be placed a drop of liquid on the crystal. ATR can be used to analyze: free-flowing aqueous solutions viscose liquids coatings Biological materials Minimal sample preparation – put the sample on the crystal and collect data Quick and easy cleaning – simply remove the sample and clean the surface of the crystal analysis of samples in their natural states – no need to heat, press or grind in pellets To collect spectra Excellent for thick or highly absorbent samples – ideal for difficult samples such as black rubber: ATR Sampling in FTIR Attenuated Total Reflection (ATR) Sampling revolutionized FTIR spectroscopy with its simplicity in sample handling and almost universal applicability. This webinar will present the theory and basic use, ideas for ATR and show many examples. Sign up for this on-demand webinar and learn more. Dr. Michael Bradley received a BS degree in chemistry from the University of South Carolina and his PhD in physical from the University of Illinois and also completed his MBA in Management. He taught chemistry for 15 years before becoming a scientific field application scientist at Thermo Nicolet, later Thermo Fisher Scientific, in 2002. Access a targeted collection of application notes, case studies, videos, webinars, and white papers Transform infrared spectroscopy, near-infrared spectroscopy, Raman spectroscopy, nuclear magnetic resonance, Uv-Vis spectrophotometry, X-ray fluorescence and more. Saliva biomarkers with reagent-free biophotonic technology have not been studied as a strategy for early detection of breast cancer (BC). Attenuated total reflection Fourier Transformation Infrared Spectroscopy (ATR-FTIR) has been proposed as a promising tool for disease diagnosis. However, its use in cancer is still beginning, and currently saliva has not been used for BC screening. We have applied ATR-FTIR to saliva from patients with breast cancer, benign breast disease and healthy, coordinated controls to investigate its possible use in BC diagnostics. Several salivary gland vibration modes have been identified in original and second derivative spectra. The absorption values at wave No. 1041 cm-1 were significantly higher () in the saliva of breast cancer patients compared to those of benign patients, and the ROC curve analysis of this peak showed adequate accuracy to distinguish breast cancer from benign patients and to eat. The band range of 1433-1302.1 cm was significantly higher in the saliva of breast cancer patients than in control and benign patients. This saliva ATR-FTIR spectral range has been pre-validated as a potential diagnostic biomarker of BC. This spectral biomarker was able to distinguish human BC from controls with sensitivity and specificity of 90% and 80% respectively. In addition, it was able to distinguish BC from benign diseases with sensitivity and specificity of 90% and 70% respectively. In short, saliva analysis by ATR-FTIR spectroscopy has shown for the first time the possible use of saliva spectral biomarkers (1041 cm 1 and 1433-1302.9 cm)) as a novel alternative to non-invasive BC diagnostics that could be used for screening purposes.1. IntroductionBreast cancer is a complex and heterogeneous disease caused by several factors, and its spread involves a sequence of clinical and pathological stages that begin with carcinoma in situ, progress to invasive lesion and culminate in a metastatic disease [1, 2]. According to the World Health Organization's 2014 World Cancer Report (WHO), breast cancer was the type with the highest incidence and mortality rate in the world's female population (1.7 million) in developing and developed countries [3]. Early diagnosis and proper treatment are the main benefits of breast cancer screening. In principle, breast cancer diagnosis includes four conventional techniques: histopathology, mammography, ultrasound and magnetic resonance imaging (MRI). In general, however, these techniques have incorrect critical limitations related to efficacy and production. or false negative results [4, 5]. Therefore, the increasing incidence of breast cancer worldwide and the lack of sufficient reliable, cost-effective and requires a search for other diagnostic tools. Attenuated Total Reflection Fourier Transformation Infrared Spectroscopy (ATR-FTIR) is a fast, non-destructive, non-invasive, label- and reagent-free, cost-effective, sensitive and highly reproducible physico-chemical tool for characterizing biological molecules in liquids. FTIR requires only a small amount of samples for analysis with easy and fast preparation, and it enables automated and repetitive analyses that lead to a non-subjective evaluation of the sample [4, 6, 7]. In addition, ATR, the experimental configuration used in this study for the detection of FTIR spectra, has a high signal-to-noise ratio (SNR), has no undesirable spectral contributions, and allows an analysis of a sample without further preparation by simply placing it in direct contact with a crystal with a refractive index higher than the sample[8-11]. FTIR can effectively provide information on the structure and chemical composition of biological samples at the molecular level and then on the characterization of proteins, lipids, nucleic acids and carbohydrates. FTIR is also sensitive to detecting changes in molecular compositions depending on the disease condition and providing fingerprints of biological samples such as tissues, cells and biological fluids. The formation and progression of malignancy at the molecular level in cells occurs before morphological changes in cancer. FTIR spectroscopy is able to show changes in carcinogenic vibration modes in several human cancers [8, 12-14]. FTIR spectroscopy was used for many purposes [15-24], mainly for detection [4, 25-28]. Most FTIR spectroscopy studies in breast cancer used normal breast tissue and breast tumors [4, 29-31], breast cell lines [11, 32, 33] and blood from breast cancer patients [25, 27]. As far as we know, there are no studies with ATR-FTIR spectroscopy for breast cancer diagnosis with saliva as a biological sample. Saliva is a complex and dynamic biological fluid consisting of 98% water and 2% of other important compounds such as electrolytes, mucus, enzymes, proteins/peptides, nucleic acids and hormones. Most organic compounds of saliva are produced in the salivary glands; however, some molecules that originate from a diseased process can be transported from the blood to the acinar lumens via transcellular or paracellular fluxes [34-36]. Then salivary gland biomarkers can be used for the early diagnosis of some systemic diseases [36-39]. Among the benefits, saliva can reflect several physiological states of the body; is easy, quick and safe to collect; is convenient to store; is not and is painless compared to blood for the patient and requires less handling during the diagnostic procedure [38, 40, 41]. Here we tested the hypothesis that certain salivary gland vibration modes can be used to distinguish breast cancer patients from benign patients and Controls that can prove that salivary gland spectral biomarkers are suitable for the diagnosis of breast cancer. In this way, the aim of the present study was to establish specific salivary gland vibration modes analyzed by ATR-FTIR spectroscopy to detect breast cancer-grade fingerprints of breast cancer suitable for diagnosis.2. Materials and methods2.1. Ethical aspects and study topicsThe study was conducted at the Federal University of Uberlandia Hospital (HC-UFU, Uberlandia, Minas Gerais, Brazil) with the approval of the UFU Research Ethics Committee (protocol number 064/2008) and on the basis of the standards of the Helsinki Declaration. All investigations were carried out in accordance with the relevant guidelines and regulations. Written consent was obtained from all participants in this study, including controls and patients, in the knowledge of the facts. The subjects were randomly selected from the population before performing routine breast cancer screening and/or surgery. The exclusion criteria were the age under 18 years, the primary tumor site outside the breast and the physical and/or mental inability to respond to the tools required for data collection. The study group included 30 subjects: 10 with confirmed breast cancer through clinical, histological and pathological examination; 10 with some benign breast diseases, such as fibroadeoma, atypical ductal hyperplasia, papilloma or others; and 10 without pathological findings, the control group. In this study, the Tumor Node Metastasis (TNM) Cancer Classification was used, which is according to the American Joint Committee on Cancer (AJCC) and the International Union for Cancer Control (UICC). This classification assesses the extent of the primary tumor (T), regional lymph nodes (N) and distant metastases (M) and provides a staging based on T, N and M [42].2.2. Sampling and preparationFor each participant, saliva samples were taken prior to surgery in Ssalivette® tubes (Sarstedt, Germany), consisting of a neutral cotton swab and a conical tube. The patient chewed the swab for three minutes, which was then returned to the tube, which was covered with a lid. Then the saliva was recovered from the swab by centrifugation for 2 minutes at 1000 × and stored at 20°C. Subsequently, the saliva samples (200 l) were lyophilized overnight. This freeze-drying of the samples removes the strong infrared light absorption of spectra, which can mask the signal from the sample and reduce the intensity of the investigated compounds [25, 43].2.3. ATR-FTIR SpectroscopySpect were used in the wave number range of 4000 to 400 cm with an FTIR spectrometer VERTEX 70/70v (Bruker Corporation, Germany) in conjunction with Platinum Platinum Platinum consisting of a diamond disc as an internal reflective element. The lyophilized sample was placed on the ATR crystal, and then the spectrum was recorded. The air spectrum was used as a background before each sample analysis. Background and sample spectra were placed in a room with a temperature 21-23°C, at a spectral resolution of 4 cm 1, and for each measurement 32 scans were performed.2.4. Spectral data preprocessingThe original FTIR spectra were normalized and the baseline was corrected with OPUS software. This software was also used to calculate the absorption of areas under spectral regions that correspond to certain saliva components, using already described parameters [43]. Second differentiation spectra from the original were performed using the Savitzky-Golay method in the Origin 9.1 software to accentuate the bands, dissolve overlapping bands, and increase the accuracy of the analysis by revealing the true biochemical properties [25, 44]. During smoothing pretreatment, the parameters of the Savitzky-Golay filter, such as the polynomial order and window points, were selected to find the relatively optimal smoothing effect. The parameters were set as 2 for the polynomial order and 20 for examined window points. The second derivative specifies negative peaks (valleys) instead of bands from the original absorption spectrum. Therefore, the analyzed wave numbers in the second derivative are the height of valleys.2.5. Statistical analysisAfter spectral preprocessing, the original and derived values were used for statistical analysis. Initially, the absorption values for certain wave numbers and spectral ranges were subjected to the normality test. The results found that parametric tests were performed for normal-distribution variables or non-parametric tests for variables without normal distribution. The specific tests are indicated on the legend of the numbers. A confidence interval (CI) of 0.95 and an alpha value of 0.05 were assumed, so that a value below 0.05 was considered statistically significant. All the tests used were two-tailed. Statistical analysis was performed with graphPad Prism versions 5.00 and 7.03 (GraphPad Software, USA).3. Results3.1. Characterisation of the characteristics of the subjects is shown in Table 1. Breast cancer, benign breast disease and control patients consisted of 10 women with an average age ± standard deviation (SD) of 53.3 ± 11.2, 41.5 ± 4.2 and 43.2 ± 16.0 years. Smoking and alcoholism patterns were similar () in breast cancer, benign breast disease and control patients. The history of smoking had a 30% incidence in breast cancer, 40% in benign and 30% under control. The family history of breast cancer was reported only in cancer patients (40%). The clinical, hormonal, diagnostic and therapeutic properties of patients with breast cancer are summarised in Table 2. CharacteristicsBreast cancer n = 10Good n = 10control n = 10age (years) Range42.0-75,033.0-49,022.0–63.0 Average ± SD53.3 ± 11,241.5 ± 4,243.2 ± 16.0History of smoking of breast cancer (%)4000Variablepatients (n = 10)N%Histological subtype Invasive ductal carcinoma660 In situ ductal carcinoma330 Mucinous Mucinous Grade G2550 G3220 NR330Primary tumor ptx110 pTis330 pT1440 pT2220Regional lymph nodes pNX220 pN0550 pN1110 p N2110 NR110Distante Metastases pM0770 NR330TNM Staging 0220 I110 II220 NR550Status ER Positive880 NR220Status PR Positive880 NR220Status HER2 Positive220 Negative660 NR220p53 Positive880 NR220Ki67 ≤14%550 >14%330 NR220Molecular Phenotype Luminal A4 40 Luminal B440 NR220Therapy Surgery (S)110 S + Radiotherapy (RT)110 S + RT + Hormone Therapy (HT)330 S + RT + HT + Chemotherapy (CT)550G1, Grade 1; G2, Class 2; G3, Class 3; NR, unreported; ER, estrogen receptor; PR, progesterone receptor; HER2, human epidermal growth factor receptor 2; p53, tumor protein p53; ki67, antigen ki67.3.2. FTIR analysis of saliva spectra between breast cancer, benevolence and control patientsThe averages of the infrared original spectrum of the entire saliva spectrum of breast cancer, benign and control patients are shown in Figure 1 with an overlay of several saliva components as proteins, nucleic acids, lipids and carbohydrates. The protein content is mainly attributed to wave numbers at 1636 cm and 1549 cm 1, which corresponds to amide I or amid E2. THE asymmetric bends of CH3 and the A-values (COO) are related to the wave numbers 1447 cm and 1404 cm 1. The wave numbers 1350 cm 1 and 1244 cm 1 indicate Amid III. The bands 1045 cm x 1 and 995 cm indicate the bands of s (PO2) or.C-O-ribose/C-C. A summary of the assignments of the main vibration modes and their respective saliva building components is in Table 3.Peak (cm-1)Proposed vibrational modeMolecular source1636Amide I ['(C=O), '(C-N), δ (N-H)]Protein1549Amide II ['(N-H') CH3)]Protein (methyl groups)1404COO- symmetrical strain

[""δ"" RNA-Uracil ring stretches nucleic acid (RNA) = strain vibrations, δ = bending vibrations, s = symmetric vibrations, as = asymmetric vibrations. The second derived infrared spectra of the entire saliva of breast cancer, benign and control patients were analyzed in detail to identify specific spectral components. The average values of the second derived infrared spectra of the saliva for each patient group are shown in Figure 2. The most important wave numbers found were found at 2964, 2929, 2875, 2659, 2358, 2322 and 2285 (3000 cm - 2200 cm, Figure 2(a)), 2059, 1635. 1544, 1450, 1404 and 1313 (2200 cm x 1300 cm, Figure 2 (b)) and 1242, 1159, 1120, 1041, 987, 877 and 613 cm 1 (1300 cm 1-600 cm, 1 region, Figure 2(c)). The vibration modes and the associated molecular sources of these wave numbers are shown in Table 4 a) b) c) a) b) c)2. Derivative tip (cm-1)Proposed vibration modeMolecular source2964CH3 asymmetric elongation (aas (CH3))Lipid2929CH2 asymmetric elongation (a (a (a acid/Lipid2875CH3 symmetric stretching (vs (CH3))Lipid2659Unassigned band 2358O=C=O stretchingCarbon dioxide2322Unassigned band 2285N=C=O stretchingNitrile2059C-N stretching of thiocyanate anions (SCN−)Thiocyanate1635Amide I (β-sheet structure)Protein1544Amide IIProtein1450CH2 symmetric bending (δs (CH2))Methylene bendingLipid and protein1404CH3 symmetric bending (δs (CH3))Protein (methyl groups)1313Amide IIIProtein1242Amide IIIPO2− asymmetric stretching (vas (PO2−))ProteinNucleic acid1159C-O stretching (v (C-O))CO–O–C asymmetric stretching (vas (CO-O-C))Protein/CarbohydrateLipid1120Phosphorylated saccharide residueMannose-6-phosphateCarbohydrateProtein (glycoprotein)1041PO2− symmetric stretching (vs (PO2−))Nucleic acid (RNA/DNA) and glycogen987C=C bendingMonosaccharides and polysaccharides877C3'endo/anti A-form helixNucleic acid613C-H out-of-plane bendingCell membranesv = stretching vibrations, δ = bending vibrations, s = symmetric vibrations, as = asymmetric vibrations.3.3. Pre-validation as diagnostic potential through ROC curve and Pearson correlationGiven the fact that sensitivity and specificity are fundamental characteristics to determine the accuracy of a diagnostic test, ROC analysis was used to determine the potential diagnosis of each vibration mode of the original and second derived spectrum. Resumption of statistical analysis (mean ± SD; t-test; ROC curve value, sensitivity and specificity) of all FTIR vibration modes of the spectra of the second derivatives (see Figure 2) are shown in Table S1 as complementary material. Here we show our results with more potential diagnoses between all analyzed bands, peak 1041 cm,1 and region between 1433 cm and 1302.9 cm. The comparison of the salivary gland vibration mode of 1041 cm x 1 in the second derivative of breast cancer, benign and control patients is shown in Figure 3. This salivary gland vibration mode has been increased in breast cancer () than in benign patients. However, this vibration mode was similar in breast cancer patients () and matched the controls. In particular, the vibration mode showed a higher absorption in breast cancer than in benign patients (), and there was no significant difference from the controls (). As expected, the oscillation mode of the salivary glands of 1041 cm and 1 was similar () in the control and the benign patients (Figure 3 letter a). Since the salivary gland vibration mode of 1041 can be used to distinguish breast cancer and benign patients, we evaluated the ROC curve and calculated the area under the curve (AUC) (Figures 3(b) and 3(c)). The ROC curve analysis shows an appropriate accuracy of the ATR-FTIR tool for distinguishing breast cancer from benign patients and control patients, with an AUC of 0.770 for breast cancer vs. control and an AUC of 0.765 for breast cancer vs. Patients. With the help of the ROC curve, it was possible to select the optimal cutoff that distinguished breast cancer patients. This resulted in a sensitivity of 80% and a specificity of 70% for breast cancer vs. control and a sensitivity of and a specificity of 70% for breast cancer vs. benign patients. a) b) c) c) a) b) c) d) Taking into account the difference between the original salivary gland spectra in the region between 1433 cm and 1302.9 cm 1, we carried out quantitative analyses in breast cancer, goodwill and control patients (Figure 4). The salivarial wave range of 1433-1302.1 cm was higher in breast cancer than in benign patients () and coordinated control patients (). It is important to note that the vibration mode was similar in benign patients and control () (Figure 4(a). Since 1433–1302.9 saliva ligament area seems to be important for discriminating against breast cancer from benign and controllable patients, we also evaluated the ROC curve between breast cancer and controls (Figure 4(b) and between breast cancer and benign patients (Figure 4(c). THE ROC curve analysis shows good accuracy of the ATR-FTIR tool for distinguishing between breast cancer and other patient groups. The AUC of 1433-1302.9 salivary ligament area was 0.835 for breast cancer vs. control and 0.770 for breast cancer vs. benign patients. Using the ROC curve, the optimal cutoff was selected, which distinguished the patient groups. This resulted in a sensitivity of 90% and a specificity of 80% for breast cancer vs. control and a sensitivity of 90% and a specificity of 70% for breast cancer vs. benign patients. a) b) c) c) a) b) c) c) 4. DiscussionOur available data support our hypothesis that ATR-FTIR vibration modes of saliva can distinguish breast cancer from benign and suitable patients. Here we have identified new salivary GLand ATR-FTIR spectral biomarkers for breast cancer screening. The oscillation mode of 1041 cm,1 salivary glands in the spectra of the second derivatives and the wave number range of 1433–1302.9 cm in the original spectra could potentially be used as salivary biomarkers to distinguish breast cancer from benign and suitable patients with very good accuracy. Our potential spectral biomarker of 1433-1302.9 cm 1 was able to distinguish human BC from controls with a sensitivity and specificity of 90% and 80% respectively. In addition, it was able to distinguish BC from benign diseases with sensitivity and specificity of 90% and 70% respectively. Considering that mammography, ultrasound and MRI, the conventional techniques used in clinical practice have sensitivities of 67.8%, 83% and 94.4%, as well as specifics of 75%, 34% and 26.4% respectively [52], we believe that our results could improve accuracy in breast cancer diagnosis. However, in order to perform traditional diagnostics, high-quality equipment and facilities are required at a significant clinical cost. In addition, circulating also used as indicators of breast cancer; However, none of them has achieved adequate sensitivity and specificity that limits their clinical applicability in breast cancer diagnosis [53]. Infrared spectroscopy enables the analysis of the entire biochemical signature (including proteins, proteins, nucleic acids and carbohydrates) of a biological sample, rather than focusing on a single specific protein as a biomarker [25]. Therefore, the salivary glands ATR-FTIR spectra are highly desirable due to their speed, convenience and cost-effectiveness, which strongly indicates this diagnostic platform for breast cancer screening. ROC curve analysis is widely regarded as the most objective and statistically valid method of biomarker performance assessment. In the current study, the ROC curve analysis showed adequate accuracy for the salivary gland level of 1041 cm-1 level of secondary-derived ATR-FTIR spectra and good accuracy for the band range 1433-1302.9. The salivary gland level of 1041 cm and 1 of the second-derived ATR-FTIR spectra was increased in breast cancer patients compared to benign patients. Surprisingly, despite the absence of significant differences between breast cancer patients and controls, this spectral biomarker candidate showed a significant diagnostic value with an AUC of 0.7700, which compares breast cancer patients as controls. In addition, it also showed a significant diagnostic value with similar AUC to compare breast cancer and benign patients. Therefore, this salivary spectral ATR-FTIR biomarker is a compatible complementary alternative to improving the diagnosis of breast cancer. The band range 1433–1302.9 was increased in the saliva range of breast cancer patients compared to control and benign patients, and this band range showed a high sensitivity and specificity to distinguish breast cancer from both controls and benign patients, as it was pre-validated by ROC curve analysis as a saliva patient ATR-FTIR biomarker of breast cancer. The discriminatory power of this breast cancer biomarker candidate reached 90% of specificity and 80% of sensitivity through coordinated controls and 90% of specificity and 70% of sensitivity of benign patients. As for the potential for use in the clinic, these data strongly suggest that the spreadof range of the region had 1433-1302.9 cm and 1, which discriminates against patients with breast cancer from healthy and benign patients. It is important to note that the saliva band area of the range 1433–1302.9 cm 1 was between benign and controllable, which is consistent with the blood test analysis [25]. It is known that increasing absorption in each specific spectral vibration mode represents an increase in the presence of a specific biomolecule [44]. The increase in absorption levels of breast cancer patients in vibration mode of 1041 cm and 1 is due to increased PO2-symmetric strains contained in nucleic acids and glycogen. Previous studies on cancer cells and tissues with FTIR spectroscopy also about many changes in the phosphate region, which corresponds mainly to nucleic acids and carbohydrates [25]. The increased content in the range 1433-1302.9 cm 1 is due to an increased CO-symmetric elongation present in proteins and lipids. Taking into account the higher expression of PO2 PO2 Stretches (s (PO2)) and COO-symmetric stretching ('s(COO)) in the saliva of breast cancer patients, we suggest that these molecules come from the blood and come to saliva through passive diffusion of lipophilic molecules (e.B.g. steroid hormones) or active transport of proteins via ligand receptor binding [35]. Therefore, saliva can represent biomarkers that reflect the pathophysiological state of the body, such as breast cancer. There are numerous supposed salivary gland molecular biomarkers that are likely to be altered in the presence of breast cancer. Higher concentrations of some proteins [54-56], carbohydrates [52] and nucleic acids [47] have already been found in the saliva of breast cancer patients compared to normal controls, which is confirmed by the results of this study. In general, these biomarkers were evaluated using proteomic, immunological and biomolecular techniques. Higher concentrations of many proteins have been observed in the saliva of breast cancer patients, such as (a) vascular endothelial growth factor (VEGF) and epidermal growth factor (EGF), which are strong angiogenic factors; (b) carcinoembryonic antigen (CEA), which is a glycoprotein and an established serum tumor marker for breast cancer [54]; (c) a soluble form of HER2 protein, i.e. a receptor tyrosine kinase, a product of c-erbB-2 oncogene and marker of poor prognosis [55]; and (d) p53, a tumor suppressor protein product of oncogene p53, regulates target genes that induce cell cycle arrest, apoptosis, senescence, DNA repair or metabolic changes, and it is the indicator of poor clinical outcome [56]. One limitation of our study is the relatively small number of patients and the need for larger multicenter studies to confirm our results. Another limitation of this study is the lack of information about the specificity of this salivary GLand ATR-FTIR spectral biomarker in breast cancer, especially considering that other cancers may also have similar changes. Therefore, further studies are needed to evaluate the diagnostic performance of these spectral ATR-FTIR biomarkers of saliva in other cancers.5. ConclusionsThe present study showed for the first time that ATR-FTIR spectroscopy can be used in saliva samples to discriminate against breast cancer patients as benign patients and healthy subjects. It was found that the absorption levels in the saliva of breast cancer patients are significantly higher than in benign patients with the wave number 1041 cm 1, and the ROC curve analysis of this peak showed adequate accuracy to distinguish breast cancer from benign patients and control patients. In addition, we have shown that the wave number of 1433-1302.1 in the saliva of breast cancer patients compared to control and benign has been increased. Our study highlighted this salivary spectrum region as a high-precision biomarker to distinguish breast cancer from both control and benign patients. In summary, these innovative results suggest that salivary gland analysis by ATR-FTIR ATR-FTIR is a promising tool for breast cancer diagnosis. Data availabilityThe data sets generated and/or analyzed during the current study are available from the corresponding author on a reasoned request. DisclosureThe donors played no role in the design of the study; in the collection, analysis or interpretation of data; in the writing of the manuscript; or in the decision to publish the results. The results presented in this manuscript are part of a patent application: Maia, Y.C. P.; Ferreira, I.C.C.; L. R. Goulart; Silva, A. T. F.; Santos, L. L. D.; Aguiar, E.M. G.; Araujo, T. G.; Sousa, L.C.; and Silva, R. S. Método para deteceó de câncer de mama baseado em componentes salivares, 2018. Registration number: BR10201801530. Receipt of payment: 26.07.2018. Conflicts of interestThere are no conflicts to declare. CreditThe authors thank the Obstetric Division of the University Hospital Uberlandia for their help in obtaining the clinical samples and the volunteer women of this study and the Research Center for Biomechanics, Biomaterials and Cell Biology of the Federal University of Uberlandia for the opportunity to use the ATR-FTIR spectrometer Bruker VERTEX 70/70v and to acquire the spectral images. This research was funded by CNPq (#458143/2014 and #449938/2014-0). FAPEMIG (#APQ-02872-16 and #APQ-01154-14); National Institute of Science and Technology in Theranostik and Nanobiotechnology - INCT - Teranano (CNPq Process No.: 465669/2014-0); CAPES and FAU - Fundao de Apoio Universitério - Universidade Federal de Uberl'ndia. Supplementary MaterialsThe supplementary material file contains table S1, which shows a CV of statistical analysis (mean r± SD; t-test; ROC Curve Value, Sensitivity, and Specificity) of all FTIR peaks of the second derived spectra shown in Figure 2. (Supplementary materials) Copyright © 2020 Izabella C.C. Ferreira et al. This is an open access article distributed under the Creative Commons Attribution License that allows unrestricted use, distribution and reproduction in any medium, provided that the original work is duly quoted. Quoted.