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ATR-FTIR spectroscopy and chemometrics as a quick and simple alternative for discrimination of SARS-CoV-2 infected food of animal origin

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HIGHLIGHTS
- ATR-FTIR spectroscopy for detection SARS-CoV-2.
- 3 min for discrimination of SARS-CoV-2 infected food.
- Minimal sample preparation and no reagents required.
- PLS-DA model led to perfect sample discrimination.

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ABSTRACT
Alternative routes such as virus transmission or cross-contamination by food have been suggested, due to reported cases of SARS-CoV-2 in frozen chicken wings and fish or seafood. Delay in routine testing due to the dependence on the PCR technique as the standard method leads to greater virus dissemination. Therefore, alternative detection methods such as FTIR spectroscopy emerge as an option. Here, we demonstrate a fast (3 min), simple and reagent-free methodology using attenuated total reflection-Fourier transform infrared (ATR-FTIR) spectroscopy for discrimination of food (chicken, beef and fish) contaminated with the SARS-CoV-2 virus. From the IR spectra of the samples, the “bio-fingerprint” (800 – 1900 cm\(^{-1}\)) was selected to investigate the distinctions caused by the virus contamination. Exploratory analysis of the spectra, using Principal Component of Analysis (PCA), indicated the differentiation in the data due to the presence of single bands, marked as contamination from nucleic acids including viral RNA. Furthermore, the partial least squares discriminant
1. Introduction

A novel coronavirus strain called acute severe respiratory syndrome coronavirus 2 (SARS-CoV-2) began circulating in Wuhan in December 2019 and a few months later gave rise to a global pandemic. This virus is the cause of COVID-19 that spreads rapidly due to its contagious nature, generating more than 510 million confirmed cases and 6 million deaths [39]. The World Health Organization (WHO) points out that the main routes of contamination are droplet transmission, contact, fomites [38]. The infection of the World Health Organization (WHO) points out that the main routes of contamination are droplet transmission, contact, fomites (contaminated surfaces) and aerosols. A global effort has been made to reduce transmission from person to person, through contaminated surfaces mainly in places with high traffic [41]. Furthermore, with the relaxing of restrictive measures new transmission alternatives have been explored, such as the possibility of food acting as a transmission agent of the virus [29]. Cases of SARS-CoV-2 have been reported in frozen foods, specifically, a case of coronavirus detected in frozen chicken wings of Brazilian origin in China [7]. This generates consumer hesitation in purchasing any raw or packaged product that may be contaminated with the virus [24]. Foodborne diseases by different pathogens such as bacteria, fungi, or viruses are a global concern as they result in about 420,000 deaths, annually, and an economic loss of approximately US$ 110 billion worldwide [40].

Rapid and early detection methods is an alternative to limit the spread of the virus, consequently increasing consumers safety and reducing the number of infected individuals. Currently the gold standard techniques for detection are polymerase chain reaction test (PCR) and enzyme-linked immunosorbent assay (ELISA), which present some disadvantages in the current pandemic scenario. PCR and ELISA tests require a high cost, specialized professionals and a long time even in developed countries take about 2 days or more. These disadvantages make them not suitable for mass testing, since despite the improvement in the scenario the pandemic was not interrupted [36].

Novel ultra-fast, selective and in-loco detection of COVID-19 are of a global effort of the researchers, industries and governments. In this context, attenuated total reflection - Fourier transform infrared (ATR-FTIR) spectroscopy can be used for this application. The FTIR technique has been applied to detect different virus Herpes [31], influenza [30], dengue [34], zika, chikungunya [35], including SARS-CoV-2 in saliva [19,25] and serum samples [44]. The vibrational spectroscopy of the infra-red region gives a profile of the virus in the bio-fingerprint spectral region [6] and a series of pre-processes were performed at a controlled room temperature of 23 °C. Before acquiring each spectrum, the ATR crystal was carefully cleaned with ultrapure water and alcohol 70 %. Spectra were collected in triplicate, and the final results were expressed as average.

2. Methodology

2.1. Sample preparation

One kg of each meat matrix: chicken breast, beef and tilapia fillets were purchased from local butchers of Rio de Janeiro City. All observable fatty parts, bones and connective tissues of the samples were removed and square sections were made to the size of approximately 1 cm². To assure the previous absence of the virus on the matrices, samples were tested by RT-qPCR, using a cotton swab to collect the material throughout the supply. Sixty samples of each matrix were prepared, 30 for reading the blank (pure) and 30 for contamination with the SARS-CoV-2 virus. The contamination was carried out in each sample by inoculating 5 µL of a solution of previously inactivated virus from nasophagel samples (Ct = 31) simulating natural contamination. Positive samples with the inactivated virus were kindly provided by the immunogenetics and molecular biology laboratory of the Hospital Geral e Maternidade de Cuiabá-MT, Brazil.

2.2. ATR-FTIR spectra acquisition

Infrared (IR) spectra were obtained using an IR Prestige-21 (SHIMADZU, Japan) FTIR equipped with a diamond crystal ATR. Spectra were acquired with 45 scans in the range 2500–650 cm⁻¹ with a resolution of 4 cm⁻¹ with 1867 data points total. Single spectra were corrected against the background air spectrum. The analyzes were performed at a controlled room temperature of 23 °C. Before acquiring each spectrum, the ATR crystal was carefully cleaned with ultrapure water and alcohol 70 %. Spectra were collected in triplicate, and the final results were expressed as average.

2.3. Spectral pre-processing and data analysis

Data pre-processing, multivariate analysis and post-processing were performed with an in-house routine implemented in Matlab® 2021a (MathWorks Inc., Natick, EUA). Before multivariate analysis, the spectra were cut from 800 to 1900 nm as referenced in the scientific literature as the bio-fingerprint spectral region [6] and a series of pre-processes were tested: standard normal variate (SNV), multiplicative signal correction (MSC), the first derivative using the Savitzky-Golay algorithm with 3rd order polynomial and 9 data-point, and the second derivative using the Savitzky-Golay algorithm with 3rd order polynomial and 9 data-point. Furthermore, prior to multivariate analyses, all spectra were mean-centered, a conventionally applied step to remove systematic bias from datasets [10].

As an exploratory unsupervised method, principal component analysis (PCA) was applied to IR spectra to reduce the dimensionality of the dataset and visualize the natural clustering of pure and contaminated samples for each meat type individually. Furthermore, the loading plot was used to verify the importance of spectral sub-regions on the differentiation among contaminated and pure samples. All scores and loads were determined using the singular value decomposition (SVD)
2.4. Classification model

For the task of supervised classification, the partial least squares discriminant analysis (PLS-DA) was implemented using the classification toolbox of the Milano chemometrics and QSAR research group [3]. PLS-DA is a discriminant technique that focus on the dissimilarities between the different classes to find class belonging traits [22].

To validate the findings of the classification model external validation was performed. For that the dataset was split into two subsets: a training set with 70% of the samples of each class (each type of meat) and a test set with the remaining 30%. The datasets were separated using the duplex algorithm [38]. Then, the validation was performed by calculating the performance parameters of the obtained classification models in terms of:

\[
\text{Sensitivity} = \frac{TP}{TP + FN} \\
\text{Specificity} = \frac{TN}{TN + FN} \\
\text{Accuracy} = \frac{TN + TP}{TN + TP + FN + FP}
\]

Where TP, TN, FP, and FN indicate the number of true positive, true negative, false-positive, and false-negative samples, respectively, and N is the total number of samples belonging to the class.

3. Results

3.1. Visual inspection of ATR-FTIR spectra

In the FTIR spectra, the signal peaks relate to the vibrations between chemical bonds and this information can be used to assign specific chemical groups to each wavelength variation, according to the literature. The main groups contained in meat matrices are lipids, amines, amides, proteins, carbohydrates, phosphates, and nucleic acids [6,32].

Fig. 1 shows the average ATR-FTIR spectra of pure beef, chicken and fish samples in the wavelength range of 400–1800 cm\(^{-1}\). The individual spectra obtained for all pure samples showed good reproducibility as shown in the supplementary material (Figure S1).

The literature assigns typical FTIR bands in existing meat samples in three main domains. The first main region comprises peaks close to 3600 cm\(^{-1}\) and to 2550 cm\(^{-1}\), coming from vibrations of lipids and proteins, with stretches mainly of N–H, and O–H respectively. On the other hand, close to 1700 cm\(^{-1}\) and 1500 cm\(^{-1}\) is the second main region, characterized by amide I bands with elongation in the C–O and C–N stretches and amide II characteristic of peptide bonds. The third region is attributed to the fingerprint of each meat, in 1450 and 600 cm\(^{-1}\), a region characteristic of several biomolecules, such as proteins, lipids, phospholipids and nucleic acids [6].

The ATR-FTIR spectroscopy technique can be an advantageous alternative for the detection of pathogens such as the SARS-CoV-2 virus when compared to the gold standard methods, PCR and ELISA. It has advantages that are necessary for the face of the current pandemic scenario, such as fast analysis, it does not require the use of reagents, which facilitates execution and lower its cost, in addition to being simple.
Table 1

| Band (cm⁻¹) | Assignment                                                                 | References |
|------------|-----------------------------------------------------------------------------|-----------|
| ~1768–1786 | methyl-esterified C=O vibration in IgG COO- group—glycosilation (IgG with sialylate N-glycans) | [21]      |
| ~1750      | lipids: ν(C=O)                                                               |           |
| ~1700–1708 | C=O in thymine                                                              |           |
| ~1600–1620 | amide I: ν(C=O)                                                              |           |
| ~1550–1560 | amide II: 3(–N–H) coupled to ν(C–N)                                          |           |
| ~1500      | in-plane CH bending vibration from the phenyl ring in phenylalanine, tryptophan or tyrosine |           |
| ~1470      | CH2 bending vibration in lipids and proteins                                 |           |
| ~1450      | methyl groups of proteins: δ([CH3]) asymmetric                              | [33]      |
| ~1400      | methyl groups of proteins: δ([CH3]) symmetric                               |           |
| ~1350      | Stretching C–O, deformation C–H, deformation N–H                             | [1]       |
| ~1165      | C–O stretching mode of C-OH groups of serine, threonine, tyrosine            | [4]       |
| ~1245      | Amide III α-helix conformation of proteins                                   |           |
| ~1250 – 1260 | amide III: ν(C–N)                                                        |           |
| ~1155      | carbohydrates: ν(C–O)                                                       | [33]      |
| ~1120      | Symmetric stretching P–O–C, phosphorylated saccharide residue                | [1]       |
| ~1225      | DNA and RNA: νs(P–O2)                                                      | [1,21]    |
| ~1030      | Stretching C–O ribose                                                        |           |
| ~1080      | DNA and RNA: νa(P–O2)                                                       |           |
| ~1030      | glycogen vibration: νs(C–O)                                                  |           |
| ~930       | Left-handed helix DNA (Z form)                                               | [33]      |
| ~971       | nucleic acids and proteins: ν(P=O4)                                         |           |
| ~960–966   | C–O, C–C, deoxyribose                                                       | [21]      |

Where: x = stretching; s = symmetric stretching; as = asymmetric stretching; and b = bending.

to handle and not requiring trained personnel. The use of FTIR for biological samples has already been investigated in the literature in the mid-infrared region (4000–400 cm⁻¹). Within this range a region called bio-fingerprint spectral was established between 900 and 1800 cm⁻¹ because it provides a large amount of information about the chemical groups present in biomolecules, serving as a fingerprint for virus [32]. This chosen bio fingerprint region is important for biological studies due to the information on molecular vibrations, including lipids (~1750 cm⁻¹), carbohydrates (~1155 cm⁻¹), proteins (amide I, ~1650 cm⁻¹; amide II, ~1550 cm⁻¹; amide III, ~1260 cm⁻¹), in addition to DNA/RNA (~1225 and ~1080 cm⁻¹) [1,21,33]. Therefore, we further analyzed the bio-fingerprint region spectral to search for distinctions between pure and spiked virus samples. Table 1 and Fig. 2 show the primary band assignment for the data set in the bio fingerprint region.

From visual analyze, the most distinctive regions between pure and spiked samples were marked in the average spectra of each food matrix (Fig. 2). The biomolecules show remarkable characteristics in the region range 1200–1600 cm⁻¹ exposing amide I and amide II bands and tend to fuse and widen mainly in liquid samples [32]. In our results, the labeling in the region of 1500 cm⁻¹ in the fish matrix and 1560 cm⁻¹ in the beef and chicken matrices was identified and assigned it as amide II protein [5,31,32]. This region was cited as a fingerprint in meat matrices [4]. The band identified in the region around 1660 cm⁻¹ was attributed to C–O lipids, which may come from the lipid bilayer known as the viral envelope in the case of enveloped viruses such as SARS-CoV-2 added to beef lipids [31].

Each of these unique characteristics arise in the FTIR spectra due to the contamination. However, this distinction often cannot be observed with visual inspection. Therefore, mathematical and statistical multivariate approaches are employed to find spectral characteristics that collectively differentiate distinct FTIR profiles.

3.2. Exploratory data analysis

As an unsupervised method, PCA was applied to FTIR spectra to reduce the dimensionality of the dataset and gain insights into the natural dispersion of the genuine and contaminated samples from each food matrix.

PCA was applied to the FTIR spectra data of each food matrix individually, and the score graph is shows in Fig. 3. For meat samples, PCA showed a well-explained variance of 83.02 % at PC1 and 13.82 % at PC2, totaling 96.84 % of the variance accumulated in the first two PCs, as shown in Fig. 3. PC1 presented 54.98 % for the fish samples, and PC2 obtained 13.82 % simultaneously, totaling 68.80 % of the total variance. While for the chicken samples, the first two PCs could explain 90.64 % of the total variance, PC1 and PC2 explained 63.97 and 26.67 %, respectively.

The supplementary material can find the loading graphs (Figure S2) for each PC in the three data sets. The information responsible for the highest weights in each PC was observed in the region between 1300 and 1800 cm⁻¹ and are listed in Table 2. The highest loading values were in the spectral bands close to ~ 1450 (characteristic of CH₃ groups of proteins), ~1500, and ~1560 cm⁻¹ (characteristic of amide II, an N–H bending vibration coupled with C–N stretching). There is still a significant weight in the regions close to ~1650 due to amide I absorption (predominantly the C=O stretching vibration), characteristic of proteins, peptides and nucleic acids [8,37].

According to Fig. 3a, PCI allowed discrete discrimination of genuine beef samples from those spiked, where most uncontaminated samples obtained negative scores on PCI (27 of 30 uncontaminated samples). In comparison, the majority of contaminated samples scored positive (28 of 30 contaminated samples). Negative scores for uncontaminated samples may be due to the lower presence of RNA that is proportional to virus levels, indicating that as samples are contaminated, they assume positive values in PCI, which characterizes an increase in N–H binding levels, coming from nucleic acids (see loadings plot, Figure S2).

An inverse behavior to that obtained for the set of fish samples compared to the meat sample is observed. In this data set (Fig. 3b), the uncontaminated samples assumed positive values, as the intensities of the characteristic bands of amide I and amide II present in the food are different when compared to the contaminated sample. Therefore they obtained the highest scores in this PC (Figures S2b and S2c), being these the variables responsible for the discrimination of fish samples in PC2.

On the other hand, a separation was not observed for the chicken samples in the scores plot technique. It can be seen in Fig. 1c that there was no formation of a well-defined group of samples in any of the selected PCs.

As PCA is an exploratory technique separation of the samples, although desirable was not the goal of the analysis. On the other hand, the usefulness of the biofingerprinting region as source of discriminant data was evidenced. Therefore, a specific classification approach was then employed. The excellent separation of classes indicates that it is possible to distinguish the spectra between genuine and contaminated matrices. This indicates that contamination with the inactivated virus induces a greater variability of data in the FTIR spectra, which allows a clear distinction between each class.
3.3. Classification PLS-DA

Classification techniques are also known as a supervised technique methods, as the algorithm learns from the training data provided before building the model to classify external datasets [10]. Among classification techniques, PLS-DA excels, as it is one of the most used classification algorithms, due to its good applicability to classification tasks of spectral data in many fields of science [6,12,14,18,42].

The PLS-DA method was used to create classification models based on the bio-fingerprint spectral region of the FTIR data, in order to discriminate between pure and contaminated samples. A model for each meat matrix was built separately, using 30 samples of pure and 30 of contaminated meat. Furthermore, the data was preprocessed by the standard normal variable (SNV) prior to modeling. SNV is a common pre-processing in infra-red spectral data, that corrects scattering effects caused by systematic bias, and factors not inherently related to the contamination effect on the samples [9].

Table 3 summarizes the classification performance of each developed

Fig. 2. Average ATR spectrum of pure (blue line) and contaminated (red line) samples for comparison. (a) beef; (b) chicken and (c) fish.
Fig. 3. Score chart for the first two principal components applied to the FTIR dataset. (a) beef; (b) fish; and (c) chicken samples.
model calculated for the training and for the test datasets. The PLS-DA presented a perfect classification for the training and test datasets, as depicted by the 100 % achieved in sensitivity, specificity and accuracy. PLS-DA is a discriminant technique focused on the dissimilarities of the classes, that works by finding a threshold that separates all the modeled classes [23,26]. Therefore, it can be inferred that the virus contamination induces a great variability in the spectral region of bio-fingerprinting spectral utilized in the model. Corroborating the study by Barauna et al. [4] who was able to detect the SARS-CoV-2 virus in saliva samples with the FTIR test. A spectral region of bio-fingerprinting 900 – 1800 cm⁻¹ was able to discriminate by the genetic algorithm-linear discriminant analysis model (GA-LDA) samples of pure saliva and contaminated saliva [4].

Furthermore, the optimum number of latent variables for each model indicates a similar complexity approach in the distinct food matrices. This can be explained by the difference in intensity in the regions that show higher PLS-DA coefficient values, for all classes, which are bands closer to 1550 cm⁻¹, which is the protein region, and closer to 1650 and 1680 cm⁻¹ that comprise proteins and nucleic acids presented in Fig. 2. Fig. 4 shows the classification performances for each pure and infected sample class in the 800 – 1900 cm⁻¹ spectra. The horizontal dashed line indicates the classification boundary between classes by assigning “+” for training, and “×” testing. Fig. 4 shows that both the training and test samples were distant from the discriminant threshold, corroborating the discrepancy found for the bio-fingerprinting region and the classification performance shown in Table 2. The good results indicate that the PLS-DA method applied to FTIR spectra is a fast and robust alternative for the detection of SARS-CoV-2 in beef, chicken, and fish food matrices. The easiness of handling, little sample preparation and fast diagnosis when coupled with PLS-DA indicates the applicability of this technique for routine operation at food facilities. Which can foment the amplification of surveillance practices, once it surpasses the shortcoming of having the production submitted to the gold standard methods, which are more laborious and expensive.

In addition, a summary of the literature on studies that used infrared spectroscopy with chemometrics for the discrimination of viruses is presented in Table 4. This technique was applied to detect several viruses, including SARS-CoV-2, in different clinical matrices (serum, blood, saliva) and cells, with only one study related to a food sample (Table 4).

As shown in Table 4, infrared spectroscopy has been widely explored as a fast and efficient alternative for viral detection. As seen in Table 4, the application of IR coupled with classification techniques leads to the excellent classification of infected viral samples, with accuracies from 92 to 100 %. In fact, the technical ability to distinguish molecular stretches has proven to provide specific and sensible information to build discriminating models. However, it is noteworthy that the application for virus detection in food matrices is still little explored, even though infra-red spectroscopy has gained a lot of applicability in the food industry majorly due to its broad applicability and current instrumentation portability [15,27,43]. Our findings have shown that although food matrices have a variable chemical composition, discrimination of infected samples can be achieved by IR spectroscopy coupled to the adequate chemometric technique, as well as cells and tissues. The only other study found dealing with a food matrix was the detection of begomovirus in papaya leaves [13], which validated findings and achieved a well-resolved separation of infected papaya leaves.

Therefore, given its remarkable capability to distinguish infected samples IR stands out as an alternative method for viral detection. Moreover, the use of IR for viral detection in food should be encouraged as this non-destructive methodology presents a direct application for in-line monitoring of viral contamination. Such routine checking is of great value for mass-testing needs, such as needed in pandemic scenarios, as for routine checking in the food industry, where food safety is of utmost importance.

4. Conclusion

The FTIR technique proved to be a viable option for detection of the SARS-CoV-2 virus in samples of beef, chicken and fish. The ATR-FTIR was shown to capture the chemical distinction caused by the viral and associated with PLS-DA was efficient for discrimination between pure and contaminated matrices. The built models showed 100 % of sensitivity, specificity and accuracy as depicted by external validation of both. Furthermore, the non-destructive nature of this technique suits it for industrial applications such as in-line routine monitoring. This study shed light on an ultra-fast alternative, with low application cost and potential implementation on food industry to prevent virus spread ensuring food safety.

CRediT authorship contribution statement

Leticia Tessaro: Conceptualization, Methodology, Writing – review & editing. Yhan da Silva Mutz: Conceptualization, Writing – review & editing. Jelmir Craveiro de Andrade: Conceptualization, Writing – review & editing. Adriano Aquino: Conceptualization, Writing – review & editing. Natasha Kilsy Rocha Belem: Methodology. Flávia Galindo Silvestre Silva: Methodology. Carlos Adam Conte-Junior:

Table 3

| Class                | Training | Test |
|----------------------|----------|------|
|                      | Number of latent variables | Sensitivity (%) | Specificity (%) | Accuracy (%) | Sensitivity (%) | Specificity (%) | Accuracy (%) |
| Chicken pure         | 5        | 100  | 100  | 100          | 100          | 100          | 100          |
| Chicken contaminated | 5        | 100  | 100  | 100          | 100          | 100          | 100          |
| Beef pure            | 4        | 100  | 100  | 100          | 100          | 100          | 100          |
| Beef contaminated    | 4        | 100  | 100  | 100          | 100          | 100          | 100          |
| Fish pure            | 4        | 100  | 100  | 100          | 100          | 100          | 100          |
| Fish contaminated    | 4        | 100  | 100  | 100          | 100          | 100          | 100          |
Fig. 4. PLS-DA prediction showing the calculated threshold for discrimination (dashed horizontal line) of (a) beef, (b) chicken and (c) fish; using the blue line for pure samples and red line for infected. The starred samples (on the right) represent the test dataset.
Table 4

| Virus             | Sample                        | Analytical technique | Method                  | Classes          | Model performance | References |
|-------------------|-------------------------------|----------------------|-------------------------|------------------|-------------------|------------|
|                   |                               |                      |                         |                  | LV | SEN | SPE | ACC |                  |
| SARS-CoV-2        | Beef, chicken and fish        | ATR-FTIR             | PLS-DA                  | Positive         | 4  | 100 | 100 | 100 | This study       |
|                   |                               |                      |                         | Negative         | 100  | 100 | 100 |     |                  |
| SARS-CoV-2        | Serum                         | FTIR                 | PLS-DA                  | Normal control   | 5   | 87  | 98  | 95  | [44]            |
|                   |                               |                      |                         | Several control  | 98  | 87  | 95  |     |                  |
|                   |                               |                      |                         | Negative         | 92  | 90  | 91  |     |                  |
| SARS-CoV-2        | Saliva                        | ATR-FTIR             | GA-LDA                  | IgG              | 99.2 | 100 | 99.6 |     | [19]            |
| SARS-CoV-2        | Saliva                        | ATR-FTIR             | MLRM                    | IgM              | 99   | 99.9 | 99.5 |     | [4]             |
| Hepatitis         | Human serum                   | FTIR                 | PLS-DA                  | Hepatitis B      | 8   | 87  | 94  | 92  | [28]            |
|                   |                               |                      |                         | Hepatitis C      | 81  | 89  | 93  |     |                  |
| Influenza         | Nasal fluids                  | Vis-NIR              | SIMCA                   | Positive         | –   | 95.24 |     |     | [30]            |
| HPV               | Cervical exfoliated cells     | FTIR                 | LDA                     | Healthy          | 98  | 98  | 98  |     | [20]            |
| Herpes            | Cell Vero                     | FTIR                 |                         | Healthy          | 98  | 98  | 98  |     | [31]            |
| Poliovirus        | Cell                          | FTIR                 |                         | Healthy          | 100 | 100 |     |     | [17]            |
| Dengue            | blood and serum               | ATR-FTIR             | PCA-LDA, GL-LDA and SPA-LDA | Infected | 100 | 100 |     |     | [34]            |
| Hepatitis C and Dengue | Human serum freeze-dried | ATR-FTIR             | PCA and PCR            | Healthy          | 100 | 100 |     |     | [2]             |
| Begomovirus       | Papaya leaves                 | ATR-FTIR and NIR     | PCA and PLS-DA          | Infected         | 99.2 |     |     |     | [13]            |
| Dengue, chikungunya and zika | Blood          | ATR-FTIR             | PCA-LDA, GL-LDA and SPA-LDA | Healthy          | 100 | 100 |     |     | [35]            |
|                   |                               |                      |                         | Dengu            | 100 | 100 |     |     |                  |
|                   |                               |                      |                         | Chikungunya      | 100 | 100 |     |     |                  |
|                   |                               |                      |                         | Zika             | 92  | 85–92 |     |     |                  |

Legend: (-) not informed; (*) visual analysis of spectra; LVs (latent variables); SEN (sensibility); SPE (specificity); ACC (accuracy); HPV (human papillomavirus FTIR (fourier transform infrared spectroscopy)); GA-LDA ( Genetic algorithm linear discriminant analysis); PLS-DA (Partial least squares discriminant analysis); SIMCA (Soft independent modelling by class analogy); MLRM (Multiple linear regression model); PCA ( principal component analysis); PCR (principal component regression); NIR (near-infrared spectroscopy).

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.saa.2022.121883.

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