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Application of spectroscopic and multispectral imaging technologies on the assessment of ready-to-eat pineapple quality: A performance evaluation study of machine learning models generated from two commercial data analytics tools

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Abstract

Recently, rapid, non-invasive analytical methods relying on vibrational spectroscopy and hyper/multispectral imaging, are increasingly gaining popularity in food science. Although such instruments offer a promising alternative to the conventional methods, the analysis of generated data demands complex multidisciplinary approaches based on data analytics tools utilization. Therefore,

the objective of this work was to (i) assess the predictive power of different analytical platforms (sensors) coupled with machine learning algorithms in evaluating quality of ready-to-eat (RTE) pineapple (*Ananas comosus*) and (ii) explore the potentials of The Unscrambler software and the online machine-learning ranking platform, SorfML, in developing the predictive models required by such instruments to assess quality indices. Pineapple samples were stored at 4, 8, 12°C and dynamic temperatures and were subjected to microbiological (total mesophilic microbial populations, TVC) and sensory analysis (colour, odour, texture) with parallel acquisition of spectral data. Fourier-transform infrared, fluorescence (FLUO) and visible sensors, as well as Videometer instrument were used. For TVC, almost all the combinations of sensors and Partial-least squares regression (PLSR) algorithm from both analytics tools reached values of root mean square error of prediction (RMSE) up to 0.63 log CFU/g, as well as the highest coefficient of determination values (R^2). Moreover, Linear Support Vector Machine (SVM Linear) combined with each one of the sensors reached similar performance. For odour, FLUO sensor achieved the highest overall performance, when combined with Partial-least squares discriminant analysis (PLSDA) in both platforms with accuracy close to 85%, but also with values of sensitivity and specificity above 85%. The SVM Linear and MSI combination also achieved similar performance. On the other hand, all models developed for colour and texture showed poor prediction performance. Overall, the use of both analytics tools, resulted in similar trends concerning the feasibility of the different analytical platforms and algorithms on quality evaluation of RTE pineapple.

Key words: pineapple, quality, vibrational spectroscopy, multispectral imaging, machine learning, SorfML

1. Introduction

In the context of tremendous technological change, a growing lack of natural resources, and a continuous evolution of consumers' life-styles and consumption habits across the globe, food industry is challenged to provide safe and qualitative food to consumers. To address the need for efficient, safe and environmental respectful production, as well as strict communication and connection with the consumers, several approaches have been developed (Nychas et al., 2016). Among these, analytical methods based on vibrational spectroscopy and hyperspectral / multispectral imaging have gained the attention of scientists, since they could fulfill the needs of food industry as rapid and efficient methods for assessing food quality (Fengou et al., 2019b; Barbin et al., 2015; Papadopoulou et al., 2011; Ammor et al., 2009; Camps & Christen, 2009), safety (Grewal et al., 2015; Brandily et al., 2011; Davis et al., 2010; Wang et al., 2010) and authentication-adulteration (Huyan et al., 2018; Ropodi et al., 2017; Suhandy et al., 2017; Jacquot et al., 2015; Ropodi et al., 2015; . In contrast with the time-consuming and expensive conventional and molecular-based techniques, the aforementioned approaches constitute a non-destructive and sensible alternative, also suitable for in-, on-, and at-line monitoring (Efenberger-Szmechtyk et al., 2018; Nychas et al., 2016; Kumar et al., 2014). Such tools have been successfully reported in the literature as promising tools for quality and safety assessment of different meat products, such as poultry (Barbin et al., 2015; Grewal et al., 2015), pork and beef (Fengou et al., 2019a; Ropodi et al., 2017; Ropodi et al., 2015; Trinderup et al., 2015; Papadopoulou et al., 2011; Panagou et al., 2014; Ammor et al., 2009; Prieto et al., 2009), as well as fish (Fengou et al., 2019b). Their application on olive oil (Guzmán et al., 2015; de la Mata et al., 2012), cheese (Jacquot et al., 2015; Subramanian et al., 2011), fruits (Liu et al., 2015; Coldea et al., 2013; Unay et al., 2011; Camps & Christen, 2009; Suhandy et al., 2009) and vegetables (Tsakanikas et al., 2018; Sravan Kumar et al., 2015; Løkke et al., 2013) has also been demonstrated at least at the laboratory scale.

It should be noted that although these instruments/approaches can be considered as efficient, the

multivariate nature of the sensor output, is rather complex and usually needs processing and/or dimensionality reduction, before the results can be interpreted (Jollife & Cadima, 2016). Nowadays, in the food sector, a plethora of machine learning approaches has been proposed by different authors in order either to predict or to quantify safety and quality of different foods using fingerprints or other 'omics' data (den Besten et al., 2018; Ropodi et al., 2016). At the same time open sources platforms are contributing in enhancing food safety management system (Tenenhaus-Aziza & Ellouze, 2015; Nychas et al., 2008).

Indeed, the need of computational tools in the area of food science /microbiology has been recognised, due to their capacity to analyse high volumes of heterogeneous data generated from the innovative technologies (Truong et al., 2019; Granato et al., 2018; Roberts & Cozzolino, 2016). This trend is clearly followed by the development of various algorithms, among others these include Ordinary Least Squares (OLS), Stepwise Linear modelling (SL), Principal Component Analysis (PCA), Partial Least Squares (PLS), Support Vector Machines (SVM), Random Forests (RF) and k-Nearest Neighbours (kNN) which can be found either in free or not commercial software with user-friendly and easy-to-use interface. However, choosing the appropriate machine learning approach based on the question that should be addressed, is often challenging and involves a comparative analysis between various algorithms in order to achieve the best possible and realistic performance. This procedure often requires strong statistical and deep interpretation knowledge (Estelles-Lopez et al., 2017).

Even though, the spectroscopic and multispectral imaging techniques have been implemented in a broad range of food products, the application of these technologies to fresh-cut and ready-to-eat (RTE) produces including pineapple (*Ananas comosus*), is limited, regardless their popularity and market value. Lunadei et al. (2011) evaluated the enzymatic browning of fresh-cut apple slices using multispectral imaging, while a second study of Lunadei et al. (2012) focused on the colour quality of RTE spinach leaves using the same analytical method. Recently, Tsakanikas et al. (2018) studied the

microbial quality of RTE green salads (rocket and baby spinach) using different non-invasive sensors based on spectroscopy. As far as RTE pineapple is concerned, only Di Egidio et al. (2009) have studied its shelf life using vibrational spectroscopy. Therefore, the aims of this work are (i) to develop mathematics models based on data derived from different analytical instruments to predict the sensory and microbial quality of RTE pineapple, (ii) to compare the models performance and assess the suitability of different algorithms and analytical platforms for monitoring the various features (iii) to explore, the capabilities and the limitations provided by each data analytical tool.

2. Materials and methods

2.1. Samples analyses

2.1.1. Sample preparation and storage conditions

Fresh-cut and RTE pineapple, packed in PVC trays (each containing 220 g of fruit), was supplied by a local manufacturer in Athens and transported to the laboratory within 24 hours from their production. The pineapples were stored in their original package at three different isothermal temperatures, at 4, 8, 12ºC and under dynamic temperature conditions (8 hours at 4ºC, 8 hours at 8°C and 8 hours at 12ºC) in high precision (±0.5ºC) incubators (MIR-153, Sanyo Electric Co., Osaka, Japan). The incubation temperature was recorded at 15-minutes intervals using electronic temperature devices (COX TRACER®, Cox Technologies Inc., Belmont, NC, USA). The sampling was conducted at regular time intervals, depending on the storage temperature, for a maximum period of 10 days. Specifically, the analyses were carried out every 14 and 10 hours ,according to the following sampling time points: 0, 14, 24, 38, 48, 62, 72, 86, 96, 110 hours, for the first 5 days and every 24 hours until the end of storage. The final time points were 230 hours for 4, 8ºC and the dynamic temperature conditions, while 134 hours for storage at 12ºC.

For each sampling time point, duplicate samples originating from the same temperature conditions but different trays were analyzed. Each sample (tray) was subjected to the following analyses: (i)

microbiological analysis and pH measurements; (ii) sensory analysis; (iii) Fourier Transform Infrared (FT-IR) spectroscopic measurements; (iv) fluorescence (FLUO) spectroscopic measurements; (v) visible (VIS) spectroscopic measurements and (vi) multispectral image (MSI) acquisition. Different pineapple parts of the same tray were used for the microbiological analysis to prevent any contamination of the samples during the spectroscopic measurements. Four independent storage experiments were finally conducted, using four different batches of pineapple. In the case of the fourth experimental replication and only for FLUO and VIS data, the corresponding spectroscopic measurements were carried out every 24 hours throughout storage. Consequently, the total number of samples for FT-IR and MSI sensors was 424, while for FLUO and VIS was 392.

2.1.2. *Microbiological analysis and pH measurements*

A 25 g portion of fresh-cut pineapple was aseptically transferred from each tray to a sterile Stomacher bag (Seward Medical, London, UK) , diluted with 225 ml of Ringer buffer solution (Lab M Limited, Lanchashire, UK) and homogenized for 60 seconds at 230 rpm in a stomacher device (Lab Blender 400, Seward Medical, London, UK). After the preparation of appropriate serial dilutions with Ringer solution, the total mesophilic microbial populations (TVC) was determined by the spread method on tryptic glycose yeast agar (Plate Count Agar, Biolife, Milan, Italy) , after incubation of plates at 25^{o}C for 72 hours. The results were expressed as the average (± standard deviation, n=8) log colony forming units per gram (log CFU/g) of fruit.

The pH values of fruit samples were measured after the microbiological analysis, using a digital pH meter (RL150, Russell pH Cork, Ireland) with a glass electrode (Metrohm AG, Herisau, Switzerland).

2.1.3. *Sensory analysis*

Two staff members evaluated in duplicate the freshness rate of three different sensory features of the samples: odour, colour, and texture. For each sensory parameter, a score was given; 1 for fresh, 2 for intermediate, and 3 for unacceptable. Finally, the samples were classified in two classes: Class 1 for fresh (or acceptable) and Class 2 for non-acceptable pineapple samples. The intermediate samples were also classified in Class 2 to simplify the pipeline process and interpretation, since the samples with score 2 and 3 were commercially unacceptable.

2.1.4. *FT-IR spectroscopy*

In parallel to microbiological analysis, FT-IR spectra were collected using a ZnSe 45º HATR (Horizontal Attenuated Total Reflectance) crystal (PIKE Technologies, Madison, Wisconsin, United States) on a FT-IR-6200 JASCO spectrometer (Jasco Corp., Tokyo, Japan) equipped with a triglycine-sulphate (TGS) detector and a Ge/KBr beamspliter. The samples were cut in small slices of such dimensions in order to cover the crystal and then, they were covered with a piece of aluminum foil. The spectral data were collected over the range of 4000–400cm^{-1} at room temperature (22 ± 2ºC), using the Spectra Manager™ Code of Federal Regulations (CFR) software version 2 (Jasco Corp.). Reference spectra, called backgrounds, were collected every 4 samples by placing the cleaned blank crystal. For both background and sample readings, 100 scans were accumulated at a nominal resolution of 4 cm^{-1}. The collection time for each sample spectrum was 2 min. At the end of each sampling, the crystal surface was cleaned with detergent, washed with distilled water, dried with lint-free tissue, cleaned with acetone and finally dried with lint-free tissue. The range 1800 and 870 cm^{-1} was finally used, since this range includes the metabolic activity of spoilage (Di Egidio et al., 2009; Ellis et al., 2002; Al-Jowder et al., 1999). Prior to further analysis, the spectral data were mean-centered and scaled (1/SDEV). Additionally, for TVC prediction, the spectra were subjected to Standard Normal Variate (SNV) pre-processing to provide the most

important information from FT-IR. On the contrary, no pre-treatments were used for sensory features.

2.1.5. *Multispectral Image analysis*

Multispectral images were captured using the VideometerLab device in 18 different wavelengths ranging from UV (405 nm) to short wave NIR (970 nm) (Carstensen & Hansen, 2003). The device has been commercialized by Videometer A/S. The spectral radiation is not continuous, but operates at wavelengths 405, 435, 450, 470, 505, 525,570, 590, 630, 645, 660, 700, 850, 870, 890, 910, 940 and 970 nm. The system is first calibrated radiometrically and geometrically using well-defined standard targets and a light setup is loaded based on the type of the product in each fresh form. The samples of pineapple were placed in a petri dish in a way that covered the entire surface and the dish was placed inside an Ulbricht sphere. The image acquisition and pre-treatment have been described previously in detail (Panagou et al., 2014) and have been implemented using the VideometerLab system software (version2.12.39). For each image, the mean reflectance spectra (along with the standard deviation values) was calculated by averaging the intensity of pixels at each wavelength. Both the mean reflectance values and their standard deviations (in total 36 features) were used for model development, as it is considered that the second ones contain relevant and important information. As it was mentioned before, the spectral data were mean-centered and scaled (1/SDEV), while SNV pre-processing was also performed for odour prediction.

2.1.6. *Visible and fluorescence spectroscopy*

The UV-VIS spectrometer used was the Hamamatsu C12880MA (Hamamatsu Photonics K.K., Shizuoka, Japan). The device has a spectral range from 850 to 340 nm and spectral resolution of 15 nm. It can be employed either for visible or fluorescence range spectroscopy by switching the mode of spectrometer and changing the settings. Specifically, the scan count was set at 10 and 3, while

integration time at 250 μs and 100.000 μs for acquisition in visible and fluorescence mode, respectively. A UV filter with 400 nm cutoff wavelength was placed in the front of the spectrometer to obtain spectra only to the visible region. Before the samples measurements, a dark calibration and a reference acquisition are performed. Dark calibration is performed with the light source off placing the spectrometer on a dark surface for both modes. The white reference was performed with the light on using a white material (in our case a folded piece of paper) for visible mode and a non-fluorescent reflective reference standard (a black plastic surface) for fluorescence mode, respectively. The samples were placed in a petri dish covering the entire surface and 10 measurements (absorbance values) were performed in different spots of each sample. The spectral values are expressed as the average of the 10 measurements for each wavelength after a normalization step. For both FLUO and VIS analytical platforms, the range 700-400nm was used for further analysis. The spectra were mean-centered and scaled (1/SDEV). Moreover, in the case of TVC prediction, FLUO spectra were subjected to SNV pre-processing, while VIS spectra to first derivative normalization with a second-order polynomial and a 9-point window. For texture prediction, FLUO spectra were also subjected to first derivative normalization with a second-order polynomial and a 9-point window.

2.2. Data analysis

2.2.1. *The Unscrambler software*

Multivariate data analysis was carried out using the data analytics software, The Unscrambler© ver. 9.7 (CAMO Software AS, Oslo, Norway). Partial-least squares regression (PLSR) was performed for the correlation between spectral data and microbial counts where, the spectral data were used as independent variables (X) and the TVC as dependent variables (Y). This method is considered suitable for spectroscopic data sets where the dimensionality problem exists (many variables but few samples) and also when the data show strong collinearity and noise (Gromski et al., 2015; Mehmood

et al., 2012; Wold et al., 2001). For sensory features, since they are categorical variables, Partial-least squares discriminant analysis (PLSDA) was performed (Barker & Rayens, 2003).

Prior to PLSR/PLSDA, several pre-processing techniques were tested on each data set with the aim to minimize any irrelevant information such as noise, particle size deviations, scattering and drifting effects (Li et al., 2018; Dixit et al., 2017; Suhandy & Yulia, 2017; Wang et al., 2015). The selected pre-processing procedure was already described in the corresponding section of each analytical method.

The data derived from isothermal storage temperatures were used for the calibration process (training set) and those derived from dynamic temperature conditions for external validation (test set). During the calibration process, leave-one-out cross validation in parallel with Martens uncertainty test was employed in order to eliminate the risk for over-fitting and test the predictive significance of the model, but also to select the significant X -variables (Wold et al., 2001; Westad & Martens, 2000). The significant independent variables were finally used for the construction of FT-IR and FLUO models for texture assessment.

The prediction performance of the developed PLSR models for each sensor was evaluated based on the following statistical parameters: slope (a), offset (b), correlation coefficient (r), the root mean square error (RMSE), the normalised root mean square error (NRMSE) (**Eq.1**) and the coefficient of determination (R^2) of the linear regression between the predicted and measured microbiological counts. For PLSDA models, the parameters for performance evaluation were accuracy (**Eq. 2**), sensitivity (**Eq. 3**) and specificity (**Eq. 4**), where positive samples are the fresh or acceptable and negative samples are the non-acceptable samples.

$$\mathrm{NRMSE} = \frac{\mathrm{RMSE}}{\max(\mathrm{DV}) - \min(\mathrm{DV})} \qquad (\textbf{Eq.1})$$

, where DV is the dependent variable (TVC).

$$\text{Accuracy} = \frac{\text{samples correctly predicted}}{\text{total number of samples}} \text{ x } 100$$

(Eq. 2)

$$\text{Sensitivity} = \frac{\text{true positive samples}}{\text{true positive samples + false negative samples}} \text{ x } 100$$

(Eq. 3)

$$\text{Specificity} = \frac{\text{true negative samples}}{\text{true negative samples + false positive samples}} \text{ x } 100$$

(Eq. 4)

2.2.2. *SorfML platform*

SorfML is a machine learning classification and regression analysis ranking system (www.SorfML.com). Specifically, it is a free web-platform able to automate the procedure of identifying the best machine learning method for comparing data from several analytical techniques and predict the freshness profiles as well as counts of microorganisms responsible of food spoilage. Using SorfML, users are able to securely upload raw experimental data collected using rapid and/or non-invasive analytical platform (e.g. Multi/Hyper-spectral imaging, Electronic nose, Gas chromatography-Mass spectrometry) in CSV format, and apply various machine learning classification and regression modelling algorithms (e.g. SVM, Neural Network, Random forests) in order to identify the best combination of analytical platform and machine learning algorithm to predict given bacterial species or quality indices. An indicative workflow of the pineapple analysis followed in SorfML is presented in **Figure 1.**

The algorithms used in this study are k-Nearest Neighbours (kNN) (Silverman & Jones, 1989), Ranger, a fast version of Random Forest (Wright & Ziegler, 2017), Linear Support Vector Machine (SVM Linear), Radial Support Vector Machine (SVM Radial) (Boser et al., 1992), PLSR (Wold et al., 2001) and PLSDA (Barker & Rayens, 2003). In order to generate each model, the dataset was randomly segmented into a training dataset for optimisation, with the 65% of the total samples, and a

testing dataset for model validation with the left 35%. The different classes of data were equally represented in training as well as testing data set. The raw data were also centered and scaled, but no other data pre-processing was performed.

The predictive power of the developed models for sensory features was evaluated based on accuracy parameter, but also sensitivity and specificity were provided. For TVC models, RMSE and NRMSE (**Eq. 1**) parameter for each analytical platform were ranked in heatmaps, while R^2 values were also presented. Training performance was assessed using *k*-repeated fold cross-validation with a k value of 4 and a total number of 10 repetitions to choose the best parameters for each model.

3. Results

3.1. *Microbiological spoilage and pH data*

The initial level of TVC (mean ± standard deviation, n=8) was 5.09 ± 0.60 log CFU/g, while the final populations were 7.14 ± 0.50, 7.69 ± 0.40, 7.52 ± 0.30 and 7.91 ±0.20 log CFU/g during storage at 4, 8, 12°C and under dynamic conditions, respectively. The growth was more rapid at the highest temperature.

No significant differences on pH measurements were found between the different temperatures and during storage. Specifically, the mean (mean ± standard deviation, n=8) initial pH value was 3.45±0.05 and the final values were 3.57±0.04, 3.55±0.07, 3.55±0.17, 3.52±0.17 at 4, 8, 12°C and under dynamic conditions, respectively.

3.2 *TVC prediction models*

Concerning TVC, the linear regression between the predicted (estimated) and the measured (observed) TVC values is presented in **Table 1** and **Figure 2** for The Unscrambler, and in **Figure 3** for SorfML. The solid lines in **Figures 2** and **3** are the ideal y=x lines, while the dashed ones determine the ±1 log unit area. Additionally, SorfML platform provides a ranking of performance

(with RMSE and NRMSE values) of the various models developed for each analytical platform and machine learning algorithm, which is illustrated in a heatmap plot (**Figure 4**). In **Table 2,** the R^2 values are also presented for each model developed on SorfML software.

Starting with The Unscrambler, the a and b values of the linear regression between the estimated and the observed TVC values have a narrow range from 0.57 to 0.61 and 2.61 to 3.00, respectively. Additionally, the RMSE and NRMSE values are quite low for all sensors. Actually, the RMSE values are close to 0.5 log CFU/g. The R^2 values are under 0.6 for all the sensors, while the r value ranges from 0.70 to 0.77. The FLUO and VIS models exhibit the highest r and R^2 values, as well as the lowest RMSE and NRMSE values. The number of components selected for each PLSR model is presented in **Table 3**.

In SorfML, RMSE values for all the studied sensors and algorithms were also below 1 log CFU/g. For almost all sensors, PLSR and SVM Linear algorithms exhibit the lowest values of RMSE (and NRMSE), with a range from 0.58 to 0.64 log CFU/g and the highest R^2 values, with a range from 0.41 to 0.50. On the other hand, Ranger, kNN and SVM Radial exhibit the highest RMSE values, above 0.65 log CFU/gr, as well as the lowest R^2 values. The regression lines between the estimated and the measured TVC values for non-linear models are not presented in **Figure 3**. The best model accuracy was achieved through the PLSR model combined with FLUO sensor, showing the lowest RMSE/NRMSE values and the highest R^2 values. The tuning parameters selected for each model in SorfML software are presented in **Table 4.**

3.3 *Sensory prediction models*

Due to the limited data used for sensory analysis, the corresponding results are presented in the Supplementary section. **Table S1** presents the number of acceptable and non-acceptable (in terms of freshness) samples for the three sensory features. It should be noted that for colour and texture, the number of fresh samples are four and three times higher than that of non-acceptable, while for odour,

the samples are more equally distributed to both classes. The prediction performance of the models developed for each one of the tested analytical platforms are summarized in **Table S2** for The Unscrambler. The accuracy ranking of models generated for sensory features on SorfML software is illustrated in **Figures S1A-C**, while **Table S3** provides also the corresponding values of sensitivity and specificity.

For The Unscrambler, none of the models reaches 90% of accuracy. The models for texture prediction have the lowest accuracy values, while for colour and odour, exceed 80% for almost all the sensors. However, in the case of colour, the satisfactory accuracy values of models are not followed by similar sensitivity and specificity values. As far as the odour prediction is concerned, , FLUO model is the only model, which has the highest values of both sensitivity (88.46%) and specificity (85.90%), and also the highest value of accuracy (86.54%) among the analytical platforms.

In SorfML, the accuracy percentage of all the models generated for all of the three features, do not exceed 89.23%. As far as the colour and texture is concerned, the models with accuracy values above 80%, show also high sensitivity and low specificity. For odour, FLUO combined with PLSDA, SVM Radial and SVM Linear, but also MSI combined with SVM Linear, show the highest accuracy values. The combinations with the best accuracy, as well as, sensitivity and specificity values are FLUO and PLSDA, together with MSI and SVM Linear.

4. Discussion

The introduction of spectroscopic and optical sensing (computer vision) methods in food science and their growing application in a wide range of food products is becoming a clear trend during the last decade. Although these analytical techniques offer rapid and in many cases efficient answers in a non-destructive way, the manipulation of the data and the interpretation of results are still a great challenge (Zhou et al., 2019).

Data analysis tools is a set of technology, that enable users to analyze and visualize data in order to identify trends and correlations with the goal of supporting decision making. Therefore, data analysis software is considered to be a central requirement for any sector / business (Vassakis et al., 2018). Although a large number of tools are available nowadays, only a limited number of these have proven to be useful for food science. The two applied statistical software, The Unscrambler and SorfML, provide a user-friendly and easy-to-use interface for analyzing large experimental datasets. These automated platforms also provide the opportunity for scientists, let alone food microbiologists with limited statistical and mathematical knowledge, to perform the challenging task of data mining and predictive modelling. However, the users are responsible for learning the advantages and the limitations of each platform and also realize that conflicting outputs are even possible (Nunes et al., 2015).

The Unscrambler software provides the option of limited in number and only linear algorithms, namely PLSR and PLSDA. On the other hand, SorfML platform offers the wide option of choosing linear and non-linear algorithms often used in data analysis. The approach of using different algorithms for the same data, allows comparing the performance of each created model and evaluate their suitability for different scenarios (Estelles-Lopez et al., 2017). Apart from algorithms, the big differences between the two data analytics tools lie on the segmentation of data in training and prediction set, the pre-processing of data and the cross-validation method.

Starting with data segmentation on The Unscrambler, the testing of the models was performed on samples stored in dynamic temperature conditions, since these data include the information from all temperatures and are also considered as a simulation of real life in the food supply chain (Tsakanikas et al., 2018). On the other hand, in SorfML, the data were randomly segmented ensuring that all temperature and storage time groups were equally represented in both data sets and finally provided a less biased selection of sample. Furthemore, using The Unscrambler, various pre-processing methods were tested and those with the best results were finally applied. The purpose was to remove

the irrelevant information from data and facilitate their interpretation. However, in SorfML, the data were subjected to the minimum treatment, with the aim not to lose important information. As far as the cross validation was concerned, leave-one-out (or full-cross) was used in the The Unscrambler, while k-fold cross-validation used in SorfML. Full-cross validation is a common method, where all samples are used in an exhaustive way providing repeatability of the results, but also may lead to over-optimistic results. On the other hand, a k-fold partitioning could result in folds where samples are not represented in an equal manner (Ropodi et al., 2016).

Besides all these different approaches, the summarized results indicate similar trends about sensors and algorithms ability to assess the quality of RTE pineapple. Specifically, for TVC assessment, all the sensors combined with PLSR algorithm show satisfactory performance in both The Unscrambler and SorfML. In The Unscrambler, the best models with slight differences compared to the others, are that based on FLUO and VIS data. In SorfML, FLUO and PLSR combination also exhibits the best performance with slight differences compared to the other PLSR models.. Apart from PLSR algorithm, it is indicative that SVM Linear combined with every sensor is also appropriate for TVC prediction. Contrarily, non-linear algorithms, tested in SorfML, do not manage to predict the spoilage of RTE pineapple.

An important observation on these results is that the R^2 values are quite low, even for the best model performances. It could be argued that according to these low R^2 values the prediction performance is poor. However, despite the widely held belief for the usefulness of coefficient of determination, there is no guarantee that a high value of this parameter is indicative of 'goodness of fit'. The value of R^2 strongly depends on the width of the prediction interval and the variability present in the data (Granato et al., 2014). In food microbiology, 0.5 log deviations are common even within the same laboratory but also, RMSE values under 1 log CFU/g, is a rather acceptable result for food microbiology applications. Moreover, the variability inside the experimental replications (batches), as well as between the two biological replicates (duplicate samples) of the same experimental

replication is too high. The latter issue is very common in plant origin products due to the strong impact of various factors such as, cultivar, geographical region, and agricultural practices.

For sensory features, the results were presented in order to reveal a potential trend which would be helpful for further investigation. The results derived from the two platforms show similar conclusions. Regarding the low number of non-acceptable over the fresh samples for colour and texture, the models generated by both software are biased over the fresh samples. Consequently, the presence of a data set with a more balanced proportion of the two classes, could possibly result in better model performances and safer conclusions for colour and texture assessment. For odour, FLUO sensor and PLSDA algorithm emerged as one of the most appropriate combinations for both tools. Additionally, SorfML software indicates that the combination of MSI and SVM Linear may be also appropriate for odour assessment in pineapple.

To conclude, the implementation of different data analytics tools requires wide knowledge of their range of applications and limitations and the results should always be evaluated critically. In this study, the results indicate that both The Unscrambler and SorfML revealed similar trends for the various analytical platforms. Specifically, the assessment of pineapple spoilage could be potentially achieved by the various types of vibrational spectroscopy (FTIR, FLUO and VIS) as well as, multispectral imaging. As far as the sensory features are concerned, the odour, could be possibly assessed by FLUO spectroscopy, conducting a more complete and representative analysis. . It is also indicative that the possibility of testing various algorithms may lead to new options and more reliable results. However, further research including feature selection analysis and data fusion strategies may be crucial in developing even more robust and accurate models (Tsakanikas et al., 2018).

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Sensor	a	b	r	RMSE	NRMSE	R^2
FT-IR	0.61	2.61	0.70	0.59	13.43	0.43
MSI	0.61	2.78	0.74	0.53	12.06	0.54
FLUO	0.59	2.96	0.77	0.51	11.61	0.58
VIS	0.57	3.00	0.77	0.51	11.61	0.58

Table 1. Performance metrics of the PLSR models, based on the different analytical platforms (sensors), for the TVC prediction of RTE pineapple on The Unscrambler software. (a: slope, b: offset, r: correlation coefficient, RMSE: root mean square error (log CFU/g), NRMSE: normalised root mean square error (%), R^2: coefficient of determination)

Sensor	Algorithm	R^2
FT-IR	Knn	0.07
	Ranger	0.16
	SVM Linear	0.42
	SVM Radial	0.12
	PLSR	0.42
MSI	Knn	0.09
	Ranger	0.13
	SVM Linear	0.44
	SVM Radial	0.12
	PLSR	0.41
FLUO	Knn	0.22
	Ranger	0.19
	SVM Linear	0.46
	SVM Radial	0.39
	PLSR	0.5
VIS	Knn	0.08
	Ranger	0.21
	SVM Linear	0.48
	SVM Radial	0.26
	PLSR	0.27

Table 2. The coefficient of determination (R^2) of the models derived from the various combinations of the different analytical platforms (sensors) and algorithms, for the TVC prediction of RTE pineapple on SorfML software.

Feature	Sensor	PLSR/PLSDA nc
TVC	FT-IR	7
	MSI	11
	FLUO	7
	VIS	12
Colour	FT-IR	7
	MSI	5
	FLUO	6
	VIS	7
Odour	FT-IR	6
	MSI	10
	FLUO	6
	VIS	7
Texture	FT-IR	5
	MSI	1
	FLUO	3
	VIS	6

Table 3. Number of latent variables for PLSR and PLSDA models developed for the TVC and sensory features prediction of RTE pineapple on The Unscrambler software.

Model	Sensory Feature	kNN	Ranger			SVM Linear	SVM Radial		PLSR/ PLSDA
		k	mtry	splitrule	min.node.size	c	sigma	c	nt
FT-IR	TVC	13	963	variance	5	1	0.03	4	7
	Colour	5	7	extratrees	1	1	0.02	1	8
	Odour	23	620	gini	1	1	0.02	128	7
	Texture	9	11	extratrees	1	1	0.01	0.25	7
MSI	TVC	17	31	variance	5	1	0.05	2	11
	Colour	23	2	extratrees	1	1	0.05	0.25	5
	Odour	11	26	gini	1	1	0.06	16	14
	Texture	15	2	extratrees	1	1	0.06	0.5	14
FLUO	TVC	33	122	extratrees	5	1	0.01	8	7
	Colour	9	67	gini	1	1	0.01	0.5	7
	Odour	17	57	gini	1	1	0.01	4	5
	Texture	11	113	gini	1	1	0.01	32	11
VIS	TVC	27	94	variance	5	1	0.02	4	6
	Colour	5	2	extratrees	1	1	0.02	0.5	5
	Odour	5	104	gini	1	1	0.02	16	11
	Texture	5	85	gini	1	1	0.02	4	15

Knn: k=number of neighbours considered,

Ranger: mtry=number of variables to possibly split at in each node, splitrule=splitting rule, min.node.size=minimal node size,

SVM: c=cost of constraints violation, sigma=scale parameter of the hypothesized (zero-mean) Laplace distribution estimated by maximum likelihood

PLSR/PLSDA: nt=number of components

Table 4. Tuning parameters used in the development of the different models for the TVC and sensory features prediction of RTE pineapple on SorfML software.

Sensor	Sensory Feature	Number of Fresh	Number of Non-Acceptable	Total Number
FT-IR / MSI	Colour	333	91	424
	Odour	147	277	
	Texture	314	110	
FLUO / VIS	Colour	314	78	392
	Odour	143	249	
	Texture	292	100	

Table S1. Total number of the measured fresh (acceptable) and non-acceptable samples for each sensory feature.

Sensor	Sensory Feature	Accuracy (%)	Sensitivity (%)	Specificity (%)
FT-IR	Colour	83.04	97.62	39.29
	Odour	76.79	50.00	84.88
	Texture	72.32	90.00	28.13
MSI	Colour	85.71	100	42.86
	Odour	83.04	61.54	89.53
	Texture	72.32	95.00	15.63
FLUO	Colour	84.62	93.67	56.00
	Odour	86.54	88.46	85.90
	Texture	70.19	90.54	20.00
VIS	Colour	81.73	98.73	28.00
	Odour	83.65	57.69	92.31
	Texture	68.27	90.54	13.33

Table S2. Performance metrics of the PLSDA models based on the different analytical platforms (sensors), for the sensory features prediction of RTE pineapple on The Unscrambler software.

Sensor	Algorithm	Sensory Feature	Sensitivity (%)	Specificity (%)	Sensor	Algorithm	Sensory Feature	Sensitivity (%)	Specificity (%)

FT-IR	Knn	Colour	91.15	10.71	MSI	Knn	Colour	95.61	46.43
		Odour	24.00	80.82			Odour	58.00	76.71
		Texture	99.06	10.71			Texture	97.17	21.43
	Ranger	Colour	92.04	14.29		Ranger	Colour	99.12	42.86
		Odour	46.00	72.60			Odour	48.00	87.67
		Texture	93.40	28.57			Texture	97.17	17.86
	SVM Linear	Colour	99.11	28.57		SVM Linear	Colour	100.00	21.43
		Odour	74.00	73.97			Odour	84.00	86.30
		Texture	99.06	17.86			Texture	93.40	32.14
	SVM Radial	Colour	97.35	10.71		SVM Radial	Colour	93.86	50.00
		Odour	36.00	75.34			Odour	50.00	80.82
		Texture	100.00	10.71			Texture	98.11	14.29
	PLSDA	Colour	92.92	39.29		PLSDA	Colour	100.00	35.71
		Odour	82.00	75.34			Odour	78.00	82.19
		Texture	96.23	10.71			Texture	91.51	35.71
FLUO	Knn	Colour	98.15	39.13	VIS	Knn	Colour	95.33	34.78
		Odour	83.67	75.00			Odour	57.14	59.38
		Texture	95.00	12.50			Texture	87.88	25.00
	Ranger	Colour	97.22	39.13		Ranger	Colour	96.26	21.74
		Odour	67.35	84.38			Odour	65.31	84.38
		Texture	97.00	29.17			Texture	92.93	25.00
	SVM Linear	Colour	100.00	26.09		SVM Linear	Colour	95.33	60.87
		Odour	79.59	90.63			Odour	73.47	76.56
		Texture	100.00	8.33			Texture	86.87	33.33
	SVM Radial	Colour	97.22	30.43		SVM Radial	Colour	97.20	34.78
		Odour	79.59	92.19			Odour	63.27	64.06
		Texture	97.00	29.17			Texture	97.98	12.50
	PLSDA	Colour	99.07	26.09		PLSDA	Colour	98.13	26.09
		Odour	85.71	85.94			Odour	81.63	71.88
		Texture	93.00	33.33			Texture	94.95	33.33

Table S3. The specificity and sensitivity values of the PLSDA models, derived from the various combinations of the different analytical platforms (sensors) and algorithms, for the sensory features prediction of RTE pineapple on SorfML software. The accuracy values are presented in heatmaps.

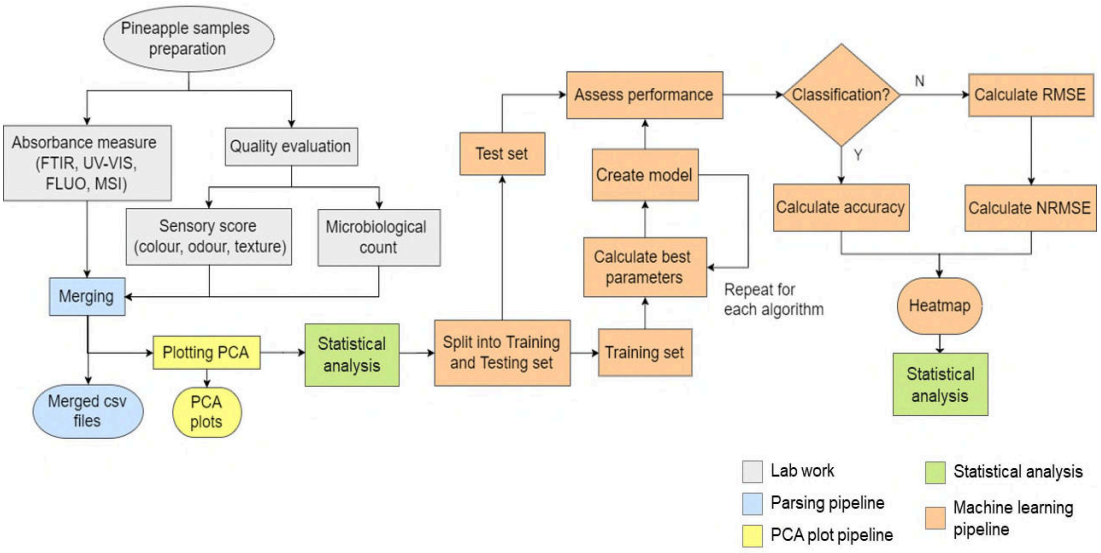


Figure 1. Workflow of SorfML. The workflow is divided into five sections with a different colour according to which part of the methodology the step belongs to.

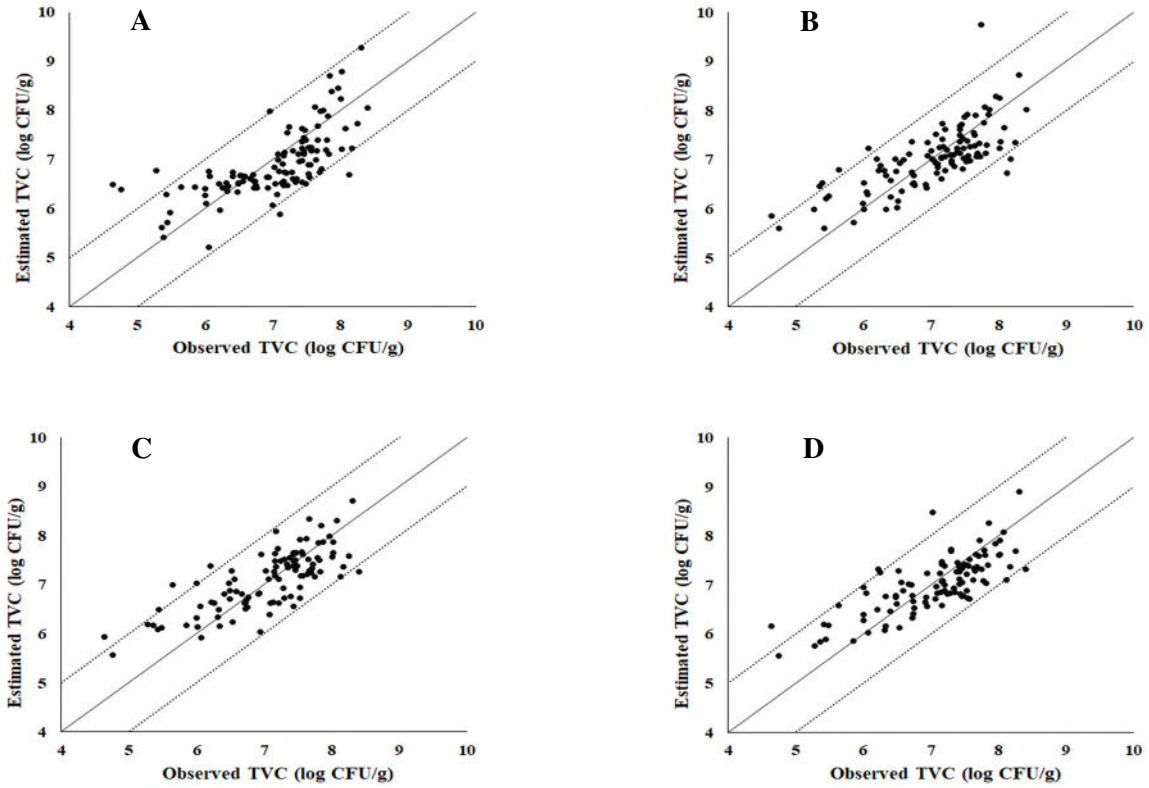
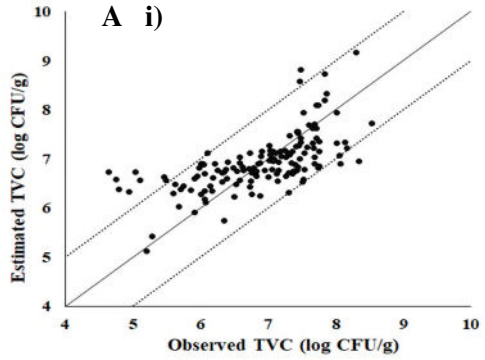
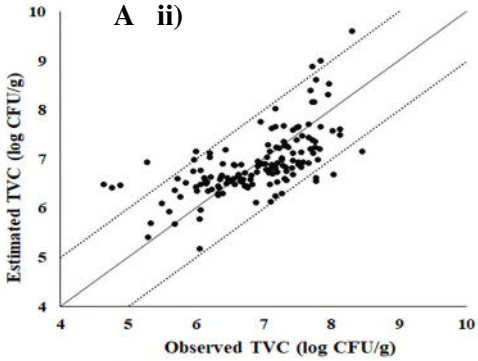
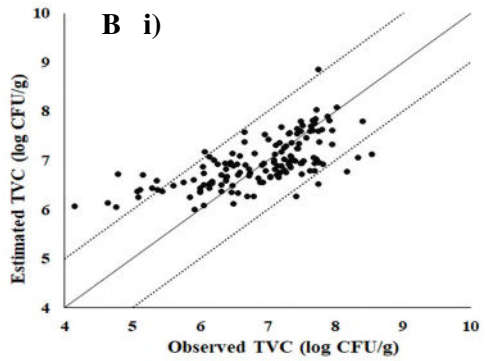
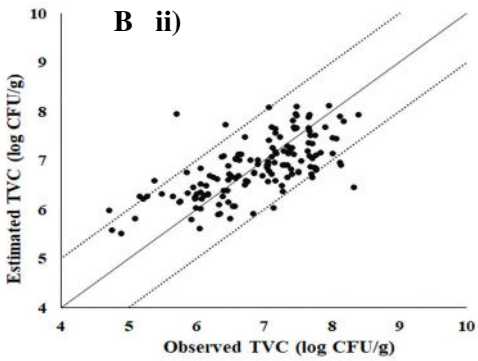


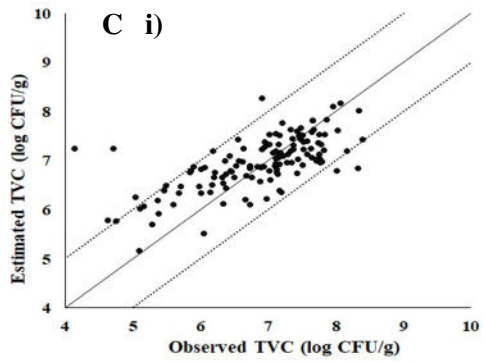
Figure 2. The linear regression between the predicted and the measured by the PLSR model TVC values of prediction based on A) FTIR, B) MSI, C) FLUO, D) VIS data for RTE pineapple, using The Unscrambler software (solid line: the ideal y=x line; dashed lines: the ± 1 log unit area).

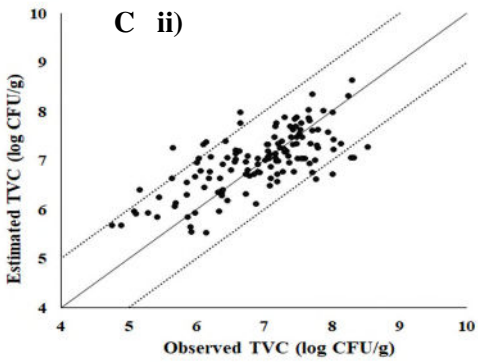

A i)
Estimated TVC (log CFU/g)
Observed TVC (log CFU/g)

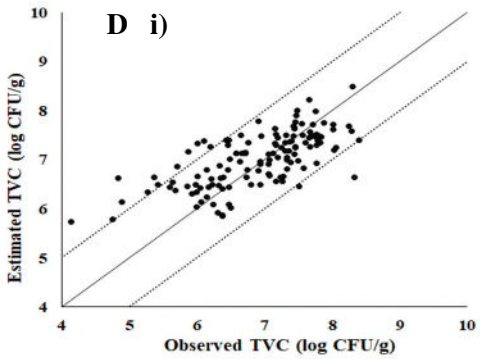

A ii)
Estimated TVC (log CFU/g)
Observed TVC (log CFU/g)


B i)
Estimated TVC (log CFU/g)
Observed TVC (log CFU/g)


B ii)
Estimated TVC (log CFU/g)
Observed TVC (log CFU/g)


C i)
Estimated TVC (log CFU/g)
Observed TVC (log CFU/g)


C ii)
Estimated TVC (log CFU/g)
Observed TVC (log CFU/g)


D i)
Estimated TVC (log CFU/g)
Observed TVC (log CFU/g)

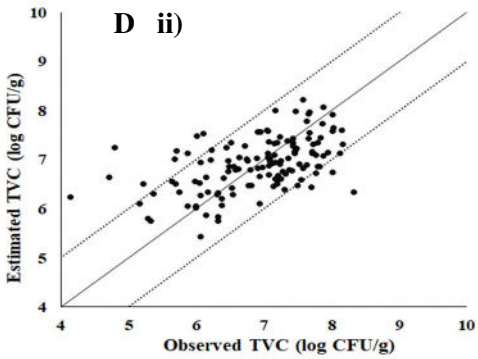

D ii)
Estimated TVC (log CFU/g)
Observed TVC (log CFU/g)

Figure 3. The linear regression between the predicted and the measured by i) SVM Linear and ii) PLSR models TVC values of prediction based on A) FTIR, B) MSI, C) FLUO, D) VIS data for RTE pineapple, using SorfML software (solid line: the ideal y=x line; dashed lines: the ± 1 log unit area).

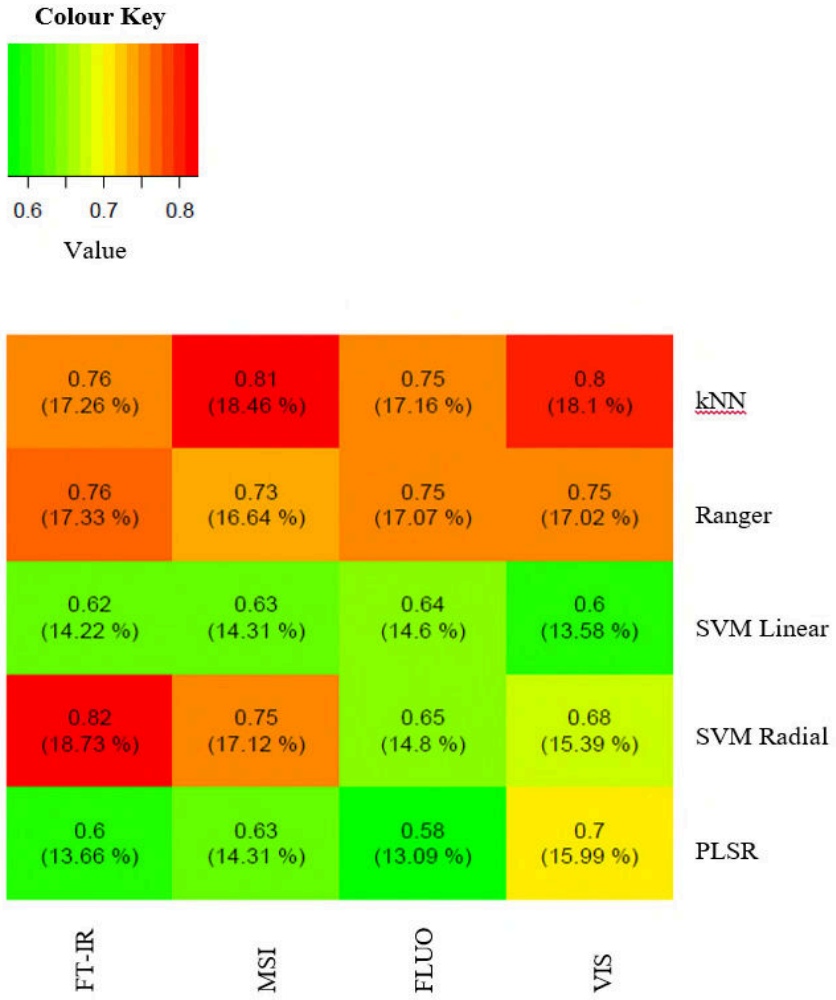


Figure 4. Performance heatmap of the different models developed for each analytical platform for the TVC prediction of RTE pineapple. In each heatmap, the rows belong to the five different algorithms, while the columns are the four different analytical platforms. The RMSE (log CFU/g) and NRMSE (%) values are presented. The colour key depicts the extreme intensity for the extreme values. The colour key begins from green (higher performance) to red (lower performance).

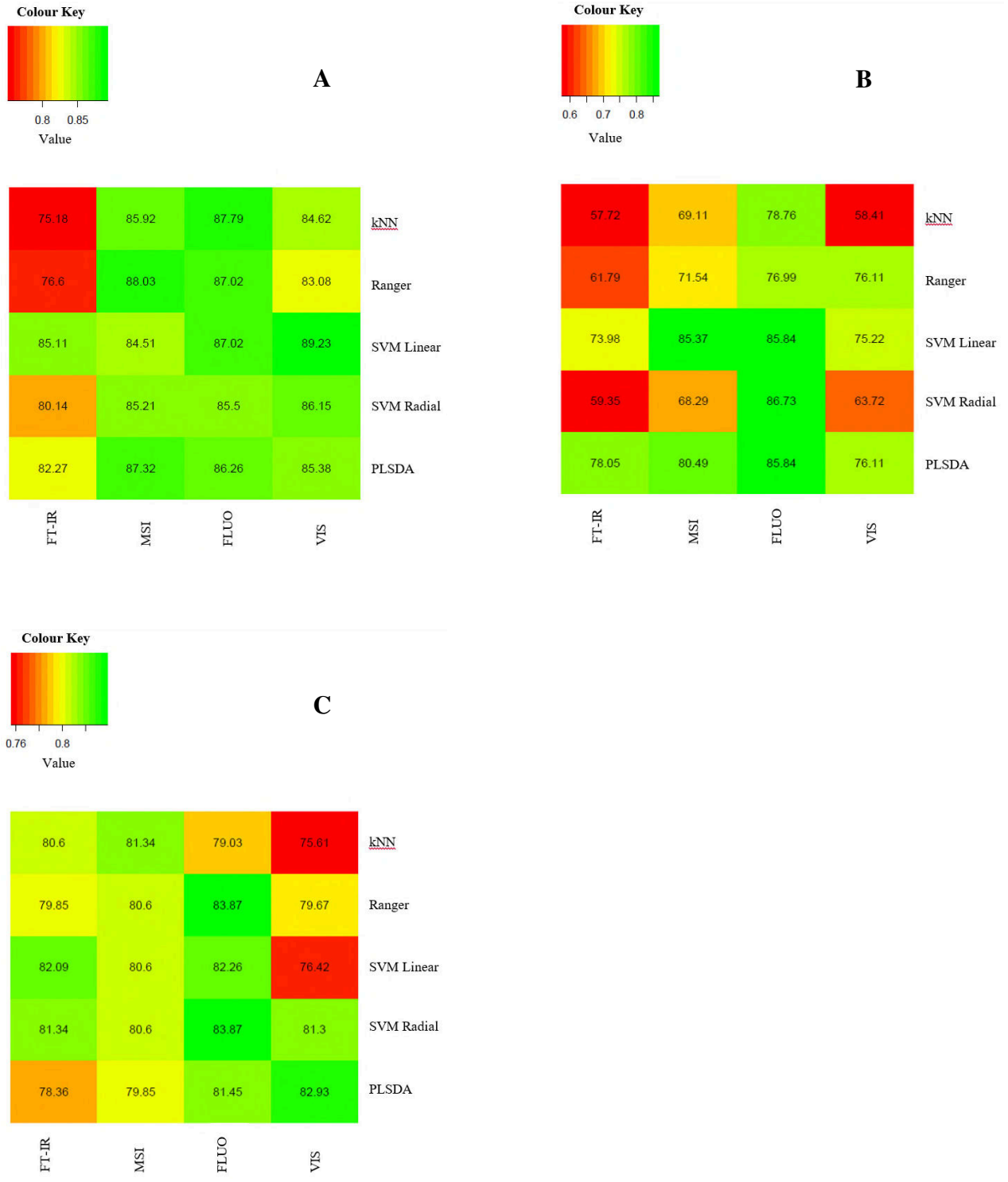


Figure S1. Performance heatmaps of the different models developed for each analytical platform for the A) Colour, B) Odour and C) Texture prediction of RTE pineapple. In each heatmap, the rows belong to the five different algorithms, while the columns are the four different analytical platforms. The accuracy (%) values are presented for the sensory features. The colour key depicts the extreme intensity for the extreme values. The colour key begins from red (lower performance) to green (higher performance).