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Acrylamide in industrial potato crisp manufacturing: a potential tool for its reduction

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Abstract

This paper considers the potential for identifying industrial manufacturing conditions that will lead to high acrylamide formation in potato crisp manufacture. Considering the available historical industrial processing data, initial tests were undertaken to identify the degree of variability and confidence in the data. Following data visualisation which indicated data 'fingerprints' characteristic of high acrylamide, Partial Least Squares (PLS) Discriminant Analysis (DA) was implemented to provide indications of the probability that high acrylamide product would be produced. It was determined that in a third of instances, high acrylamide could be predicted while maintaining a low level of false predictions. The predominance of fructose concentration in the prediction along with the need for asparagine were indicated and aligned well with prior literature mechanistic model indications. The ability to identify a third of high acrylamide occurrences provides the process operators with a good opportunity to make process modifications that would comply with increasingly stringent regulation.

Keywords

Acrylamide; crisps; Food Processing; Maillard Reaction; Partial Least Squares

1. Introduction

Acrylamide (ACR) is a product of the Maillard Reaction, which occurs when foods containing protein and reducing sugars are heated to high temperatures (Parisi and Luo 2018). The formation of ACR during cooking and/or processing was first reported in 2002 by the Swedish National Food Administration (SNFA) and the University of Stockholm (Tareke, Rydberg, Karlsson, Eriksson, & Törnqvist, 2002).

ACR is a known carcinogen in rodents (Friedman, Dulak, & Stedham, 1995; Capuano & Fogliano, 2011) which has led to its classification as a probable human carcinogen by the International Agency for Research on Cancer (1994).

The European commission has set benchmark levels of ACR acceptable to find in manufactured and processed foods. For potato crisps the indicative value was set at 750 µg/kg in 2018 (Commission European, 2017). For food production this means having a clear understanding of the amount of ACR in their products but also having an appreciation of raw material characteristics and processing operations that lead to increased levels. FoodDrinkEurope have published a toolbox which outlines process changes to be adopted by manufacturers to reduce the formation of ACR in food (FoodDrinkEurope, 2013). Within the European Union, a more formalised requirement was put in place with Commission Regulation (EU) 2017/2158 that came into force in April 2018 that required companies to take mitigation measures and track success via routine measurement. The guiding principle behind this is, by applying best practice in operation, a reduction in ACR will follow. Notably it is stated that '*the level of ACR in 10 % to 15 % of the production with the highest levels can usually be lowered by applying good practices*'. Food business operators are expected to implement measures to reduce ACR in their final product to a level "As Low As Reasonably Achievable" (ALARA), including a risk-benefit analysis. Namely a mitigation strategy that reduces ACR at the detriment of the overall nutrition of the product is not a desirable outcome (Seal et al., 2008).

ACR formation, quantification (Elbashir, Omar, Ibrahim, Schmitz, & Aboul-Enein, 2014) and mitigation (Vinci, Mestdagh, & De Meulenaer, 2012; Salazar, Arámbula-Villa, Hidalgo, & Zamora, 2012) has received significant research subsequently.

The formation of ACR requires asparagine and reducing sugars, and is affected by time, temperature, pH and moisture (De Vleeschouwer, Van der Plancken, Van Loey, &

Hendrickx, 2008a). The kinetics of the formation of ACR has been investigated extensively in model systems (De Vleeschouwer, Van der Plancken, Van Loey, & Hendrickx, 2008b; Knol, Linssen, & van Boekel, 2010; Knol, van Loon, Linssen, Ruck, van Boekel, & Voragen, 2005a).

There has been much research into the mitigation of ACR formation for potato crisps. Strategies includes selection of potato variety (Elmore, et al. 2015), inclusion of additives in the hot wash such as acids (citric acid) (Kita, et al. 2004), salts ($CaCl_2$) (Mestdagh, et al. 2008) or enzymes (asparaginase) (Pedreschi, et al. 2011), monitoring of the colour (Serpen and Gökmen 2009) and controlling the fryer conditions (Matthäus and Haase 2014). Mitigation strategies tested at laboratory scale, when scaled to industry the reduction in ACR is reduced. It is also important to note that these studies analysed crisps that have both a flat shape and uniform thickness, and that crisps with a varying thickness and ridge shape (as in this case study) are affected differently by the treatments.

Predicting and preventing the formation of acrylamide, opposed to detection following formation is preferable to the food industry. Segtnan et al. modelled ACR formation using multiple linear regression (MLR), partial least squares regression (PLSR) and design variables to identify the key parameters affecting ACR formation in crisps (Segtnan, Kita, Mielnik, Jørgensen, & Knutsen, 2006). Knol and co-workers employed empirical models and logistic exponential models to ACR formation and found the logistic-exponential model initial reducing sugar concentration and parameter a, to be most promising, however the predictive capacity of the model was not tested extensively (Knol, Viklund, Linssen, Sjöholm, Skog, & van Boekel, 2009).

This paper describes a study that considered data currently available from a production-line making crisps, to better understand factors arising that cause high acrylamide. With such understanding, operators can act in a more informed manner on the processing conditions to

reduce ACR formation. It is argued that since this study only considered data that is routinely available, this falls within the ALARA requirement. A critical consideration is that in reviewing historical data is it possible to ascertain the percentage instances of high acrylamide, it is explainable and whether they exceed the 10%-15% EU regulation aim. If so then the scope for achieving reduction beyond EU regulation targets is achievable. In this paper we use industrial production line data alongside pre and post testing for initial reducing sugars concentrations and ACR content as inputs for partial least squares regression analysis (PLS). Data from one year was used as a training set and a subsequent year as a validation set.

2. Material and methods

2.1 Chemicals

Methanol (LC-MS grade), acetonitrile (HPLC), hexane (HPLC grade) and sodium chloride (NaCl, 99.5%) were purchased from Fisher Scientific. Magnesium sulphate ($MgSO_4$, 97%) was purchased from Acros Organics. Primary Secondary Amine sorbent (PSA) was purchased from Agilent Technologies (CA, USA). Acrylamide (98%) was purchased from Fluka. [2,3,3-d_3]-acrylamide (98%) was purchased from Sigma Aldrich (UK). D-fructose, D-glucose, sucrose (Total Glucose) and L-asparagine/L-aspartic acid (system reagents) were purchased from Thermo-Scientific.

2.2 Production line data collection

For each sample the potato variety, initial glucose, fructose, total sugars and asparagine concentrations were recorded. The potatoes variety used were *Lady Claire* and *Taurus*. From the production process, line number, fryer temperature (inlet and outlet), hot wash

temperature and moisture content were recorded on-line. Final ACR content determined off-line.

Data was collected over a period of 30 months from the manufacturing line of KP Snacks from late 2016. While more than one line is used to produce the product of interest, only one line was considered to remove between line variability. On-line data was recorded 1/minute. Off-line data determination (ACR and potato composition) varied in frequency with 1/day being typical. ACR was quantified by LC-MSMS. Glucose, fructose, sucrose and asparagine concentrations in the potatoes was quantified by Konelab (Arena 30).

2.3 Precursors analysis

Precursor analysis was performed as the potatoes arrive on site with a 27.5 tonne load typically processed within 24 hours of arrival. The load composition was determined to be stable for the duration of processing period.

The analysis approach involved taking a subsample of 5 kg which was washed and blended for initial analysis. Glucose, fructose, total sugars and asparagine were measured using the Konelab 20 biochemical analyser (Thermo Fisher Electron Corporation, Courtaboeuf, France). Blended potato (50g) was mixed with 50mL of water. Carrez 1 and 2 (4 mL of each) and octanol (2-3 drops) were added and the solution homogenised. The sample was diluted to 250 mL, allowed to stand for 10 minutes then filtered. The filtrate was analysed with the Konelab analyser. The accuracy of the results was determined by processing five replicate samples of the same stabilised solution, using potatoes of different varieties and sugar content. The average confidence boundary is displayed in Table 1, showing the method accuracy according to Friedel et.al. (2013).

2.4 Acrylamide analysis

ACR quantification was carried out using the three-phase extraction method described by Mastovska & Lehotay (2006) with modifications. Briefly 1 g of blended fried crisps was combined with [2,3,3-d_3]-acrylamide (10 µL, 0.2 mg/mL), 10 mL water, 10 mL acetonitrile and 5 mL hexane, 4g MgSO4 and 0.5 g NaCl. The mixture was vigorously shaken for 1 minute and then centrifuged (5000 rpm for 10 mins). One ml of the acetonitrile layer (middle layer) was transferred to a 2ml Eppendorf tube containing 50 mg of PSA and 175 mg of MgSO4, this was vortexed for 1 min and centrifuged (1000 rpm for 1 min). The supernatant was transferred to a HPLC vial for analysis by LC-MS/MS.

ACR quantification was performed on a Thermos Fisher Scientific, San Jose, CA, USA) consisting of a degasser, a quaternary pump, a thermostatic autosampler, a column oven and a TSQ Mass spectrometer. Chromatographic separation was achieved with ultra-pure water containing 0.1 % formic (mobile phase A) acid and methanol containing 0.1 % formic acid (mobile phase B). The gradient was 98% A at 200µl/min for 3.5 min, the flow rate increased to 300 µL/min and 75% B over 2 mins and held for 2 mins before re-equilibration to initial conditions for 16.7 mins. Sample (10µL) were injected on a Synergi Hydro RP column (250 mm x 4.6 mm x 4 µm, 80 Å pore size) (Phenomenex, UK).

The mass spectrometer electrospray ionisation (ESI) in positive mode. Multiple reaction monitoring (MRM) transitions were m/z 72.07→55.1 and 44.0 for ACR and 75.2→58.0 and 44.0 for 2,3,3-d_3]-acrylamide (Internal standard) with a dwell time of 100 ms. The MS source conditions were spray voltage 3500 kV, capillary temperature 270 °C, nitrogen was used as a nebulizer gas. ACR and the internal standard eluted from the column at 2.8 mins. ACR was quantified using a linear calibration with a 1/x fitting with a range 10-1000 ng/mL ($r^2 > 0.99$), with a method detection limit of 26.7 ppb (equivalent to 267 µg/kg).

2.5 Crisp Processing Line

149 The crisp processing follows a standardized protocol. The ACR precursors were analysed
150 during storage (Figure 1) following different unit operations they reach the fryer, temperature
151 of the oil was monitored and taken into consideration on the PLS analysis as well as the off
152 line ACR measurements values. Following a system engineering approach to assess the line
153 behaviour it is necessary to understand the fundamental reactions occurring during the
154 process as far as possible, the behaviour of the processing plant and operators and the
155 variability that can occur within a factory scenario. Previous kinetic studies tackled lab scale,
156 not considering the added complexity of a food processing plant. This study aimed to build a
157 predictive tool applicable in factory settings using food factory data.
158

159 ### 2.6 Statistical analysis

160 Principal Component Analysis (PCA) was carried out using the PCA toolbox for Matlab as
161 described by Ballabio (2015). The PLS-DA was performed using the Classification toolbox
162 for Matlab as described by Ballabio and Consonni (2013). ACR analysis was performed in
163 order to consider biological and technical repetition (four observations per sample). The
164 analysis was carried out using Matlab R2018b.
165

166 ## 3. Results and discussion

167 In analysing system data it is important to build on qualitative and semi-quantitative
168 understanding of the underlying system to underpin and verify the results provided by the
169 data analytic methods. Prior fundamental knowledge of reaction mechanisms and their
170 drivers is thus important in assessing the results

171 ### 3.1 Implications of known reaction mechanisms

172 It is widely known that the initial step of the Maillard reaction is between a reducing sugar
173 and any amino acid (or nitrogen source) and that it occurs more rapidly with fructose than

glucose (Dills Jr, 1993) and that the open chain form of both are necessary for this reaction. The resulting Schiffs base rearranges to give either an Amadori rearrangement product (ARP), from glucose or a Heyns rearrangement product (HRP), from fructose. These dehydrate and fragment, regenerating the free amino acid and forming a group of highly reactive dicarbonyl compounds, deoxyosulose, dicarbonyl, and hydroxycarbonyl (Figure 2). These intermediates undergo a classical Strecker degradation with an amino acid to form flavour and colour compounds (Mottram, Wedzicha, & Dodson, 2002; Wedzicha, Mottram, Elmore, Koutsidis, & Dodson, 2005).

The importance of temperature controlling the rate of reaction from fructose to ultimately ACR was reported by Knol *et al* (2005b) and the activation energy as considered by Parker *et al* (2012). According to Knol, above 160^{o}C the rate constant to convert glucose to fructose increases significantly. The increasing of temperature impacts also on rate constants between reactants where the reaction of asparagine with fructose is preferred, compared to the reaction with glucose (at temperature >140^{o}C).

The impact of temperature on rate of reaction is shown in Figure 3. Figure 3a shows the experimental data fit and Figure 3b is expanded to highlight the typical range of temperatures experienced in the production fryer. The implications of this from an industrial operational perspective are that for the temperature range of the fryer (150^{o}C to 170^{o}C) there is a four-fold increase in rate constant, clearly demonstrating tight control of the fryer temperature is vital if ACR is to be reduced.

3.2 Initial data screening and Pattern Recognition

Once the variability of individual samples was established, the next step was to understand the behaviour of the important process inputs and outputs to appreciate the breadth of operation and where possible quantify the distribution characteristics. Visualisation of the

distribution additionally highlights potential outliers and verifies the data validity of those samples. Before plotting the data distributions as shown in Figure 4, a number of outliers were removed, that were due to human entry errors (for example, data a factor of 100 out due to decimal point errors), training set n=111, test set n=111. In Figure 4 all the data available over the two-year period of operation is considered. Such plots are useful to consider both at an early stage of analysis to understand the extent of variation but also subsequently, once the impact of variation is clearer.

Crucially important is the assessment of the ACR variation in the product as shown in Figure 4. Here a normal distribution and non-parametric distribution have been fitted to the data using the Matlab Statistics toolbox. As expected the data is not normally distributed and the fitted standard deviation of 290ppb over-estimates the extent of variation and a mean of 560ppb over-estimates the mean operating value. The cumulative probability density function of the non-parametric fit (not shown) indicates a 50% probability at 490ppb and a 93% probability of being less than 1000 ppb

Applying Parallel Coordinates Analysis as shown in Figure 5, allows a useful visual approach to gain initial insight into the relationships within the data set.

The parallel coordinates plot takes process values, applies auto-scaling to each variable and plots each variable position on the Y-axis scale. For each time point, the values of all variables are joined by lines. The utility of the parallel coordinates plot comes from the colour coding strategy, where, in this case the variable on the far right, ACR concentration is colour coded based on magnitude. In this case four colours are chosen, below the 750ppb threshold, between 750ppb and 1000ppb legal threshold and two that are greater than 1000ppb. The spread of colours found for fryer inlet temperature shows no high ACR is found below 170^{o}C and fryer outlet temperature is below 153^{o}C. Above those temperatures a mix of colours is observed but without a clear pattern, so these temperatures alone do not lead

to high ACR. For precursors, glucose, fructose and asparagine, a colour pattern is more apparent for high ACR. Variety indications are that *Taurus* (the third node in the plot) typically leads to higher ACR than other varieties. Typically in such analysis, a clear single variable to variable of interest relationship is not observed, but several variables are indicated as having some impact.

An interesting observation relating to online colour measurement is apparent. While the literature suggests that the 'A' value correlates to ACR (Gökmen, Açar, Arribas-Lorenzo, & Morales, 2008), the online measurement indicates some correlation to high ACR but it is not sufficiently sensitive in the industrial environment to distinguish by itself as a surrogate measurement of ACR.

3.3 Principal Component Analysis

In analysing the behaviour of a system, the ultimate objective is improving control, the first step is typically to apply Principal Component Analysis (I.T., 2002). The purpose of PCA in this case is to compress high dimensional process data into a low dimensional graphical representation that allows 'abnormal' conditions to be identified and the combination of process variables that cause them to be indicated as 'abnormal' to be determined. The compressed information can then be interrogated to assess deviations from standard or desired behaviour. The compressed information forms new 'variables' – the principal component scores, which are weighted summations of all the original process variables. Patterns are identified in the scores plots to detect deviations from typical behaviour. In this case process data from samples where ACR was less than 750ppb were used to generate the PCA model (class 1). The inputs used are the same as those considered in the parallel coordinates with the exception of potato variety which cannot be quantified. Subsequently

data from, higher than 750ppb ACR (class 2), was plotted on the same scores plot. Figure 6 shows scores plot for PC1 against PC2 generated.

It is observed that the points corresponding to higher ACR are shifted towards the right hand side of the plot compared to the blue, lower ACR blue points. The important interpretation from this plot is that there are combinations of variables that are in the data that are descriptive of different levels of ACR given the varying location in the scores plot. In this case, the two PC's explain 39% of the overall data variance. While this is less than half of the overall variance, the key finding at this stage of the data analysis is that there are patterns in the data that indicate information is present to distinguish high and low ACR. This therefore suggests that the information could be used for predictive modelling purposes. In the subsequent modelling of the data, in Section 3.4, considerably more of the data variance is used to build the model. It is important to realise that while patterns are apparent in the PCA plot, the quality, capability and reliability of the model can only be judged on the model itself, with PCA indicating potential but it is not an end in itself.

3.4 Acrylamide Prediction

The aim of the modelling task is to provide the plant operators with a warning that characteristics of the potatoes have an increased probability of high ACR in the final product, thus allowing process adjustments to mitigate ACR formation. For the process operators a 'traffic light' warning system would be the simplest to interpret and react to.

Given this requirement the modelling tasks requires prediction of membership of a class (high ACR or not) based on the variables available to them at that time. This classification task is firstly tackled using PLS-DA. Given that the operators need to predict, then the variables available to them for the prediction becomes a subset used in the pattern recognition task. Hence the use of precursor concentrations and fryer temperatures. PLS-DA analysis is

first considered on all the samples available from the production line. Subsequently, only the most common variety is considered to investigate whether variety has an impact on predictability.

3.5 PLS Discriminant Analysis

The development of the PLS algorithm to perform discriminant analysis was described by Barker and Rayens (2003). Lee *et. al.* (2018) presents a review on the use of PLS-DA and the practices that need to be adopted for its effective implementation. Here the PLS-DA algorithm attempts to determine the probability that a sample belonging to either low ACR or high ACR classes. Data from 2017 and 2018 were available. A common approach in model building is to randomly sample from the available data to create model building and validation sets. In this case, if inter year variation exists then this may act to mask intra year variation. Furthermore, from a practical perspective, models are built on available data and used on new data as it arrives. Thus, rather than randomly sampling, using data from 2017 to construct the model and data from 2018 to test the model was considered to be more realistic and appropriate. In Figure 7a, the circles represent the probability that a sample will result in high ACR (class 2) for 2017 model building data and the stars denote 2018 testing data. The clusters around 70 and 180 samples are the processing of new potato crops when ACR tends to be low. Figure 7b shows the model coefficients for the PLS-DA model. It is interesting to observe the significant impact that fructose and asparagine have on the likelihood of high ACR. As expected, glucose is observed to have little impact whereas sucrose has a negative impact. This negative impact arises as high sucrose is characteristic of the new potato crop, low sucrose (high fructose) is typically observed when sucrose is converted to reducing sugars by cold-induced sweetening (Sowokinos, 2001).

To use the information provided by the model, a boundary needs to be drawn in, probability, above this threshold, predicts high acrylamide. The approach within the PLS-DA toolbox is to set the threshold to reduce the incidence of misclassification. While this is theoretically acceptable, in an industrial setting if actions are taken that have cost implications then the cut-off that minimises misclassification is not necessarily the most appropriate. Table 2 considers the impact a threshold of probability has on the misclassifications of high and low ACR on the 2018 testing data. It can be seen, that if a probability threshold is set at 0.75 roughly half of those potatoes that result in high ARC are identified. However, for the 13% of potatoes that are incorrectly predicted as being high ACR, costly actions to mitigate ACR formation could be unnecessarily implemented. By increasing the threshold to 0.95 this misclassification problem can be reduced to 7% but at the expense of now only identifying around a third of the high ACR occurrences. Of the 7% misclassification, around half of those lie in the 600-750ppb ACR range so some degree of action would be appropriate. Further industrial considerations are thus required to specify the appropriate location of the threshold taking into account process costs.

4. Industrial Implications of the Results

Given recent EU Regulation, the onus is on companies to take actions to attain ACR concentrations that are ‘ALARA’ with the target set to reduce concentrations in the top 10% - 15% of cases that violate guidance levels. To understand the scope of these targets it is necessary to understand the performance and causes of high ACR as far as possible in the process. The industrial collaborator had two years of raw potato and product compositions logged on a routine basis to facilitate the assessment. Firstly, it was important to understand the accuracy of the information provided in testing and the representative nature of a sample

from a potato load. It was found that while the errors were not insignificant, they were accommodated by adopting an internal target of 750ppb as opposed to the EU guidance of 1000ppb.

Analysis of the data routinely logged using data visualisation and pattern recognition techniques demonstrated relationships were present in the data that could distinguish the likelihood of high ACR in many instances but quantifying the percentage required more detailed analysis. From an operator's perspective, a 'traffic light' system that warns of potential issues with ACR based on current line settings and potato characteristics was thus sought. PLS-DA was found to perform well in extracting the patterns contained within the data, although further process consideration based on plant costs is required to set the 'optimal' choice of threshold of probability. Interestingly, the predominance of fructose concentration in leading to the formation of ACR in the industrial production was in agreement with existing mechanistic models (albeit those considering French fries) and questioned the factory standard approach of considering the total reducing sugar concentration. The 30% detection rate demonstrated aligns well with the EU regulation targets of 10-15% of samples need to be reduced. The challenge resulting or the operators is if 30% can be detected, can process conditions be modified to act effectively on half of those being highlighted. Through more rigorous attention to fryer temperature control and the effective use of the hot-wash to reduce sugar levels prior to the fryer it is hoped that this is achievable. Work is currently addressing the control strategy, progressing the detection studies reported in this paper.

Finally, while the PLS-DA technique is implemented without considering potato variety clearly varieties have different precursor concentrations and behave in a different manner.

Initial analysis showed no benefit to variety specific models, due to limited data sets, further process data is required to verify this finding

5. Conclusion

This paper has considered the variations in ACR concentration that arise in the industrial manufacture of crisps. Analysis of available data from the manufacturing line has been shown to provide insight into the causes of high ACR in 30% of the instances that arose. These findings have focused the attention of operational staff on specific aspects of the production line to allow action to be taken to address these known causes and achieve a reduction in ACR levels. Importantly also, the analysis has suggested that 70% of the high ACR values were not explainable by the available data. This finding has initiated an industrial improvement programme focusing on unit behaviour, information availability and measurement accuracy to reduce instances where high ACR occurrences arise for unknown reasons and is the first step in further reducing the frequency of high ACR.

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Figure 1 – Unit operations in the industrial production process of crisps

Figure 2 – Reaction scheme for the formation of acrylamide. Adapted from Parker, Balagiannis, Higley, Smith, Wedzicha, & Mottram, 2012

Figure 3 – Impact of temperature on the rate of reaction of asparagine and fructose to acrylamide a) 120-200 °C b) 150-170 °C

Figure 4 – Frequency distributions for acrylamide and inset sucrose, glucose, fructose & asparagine,

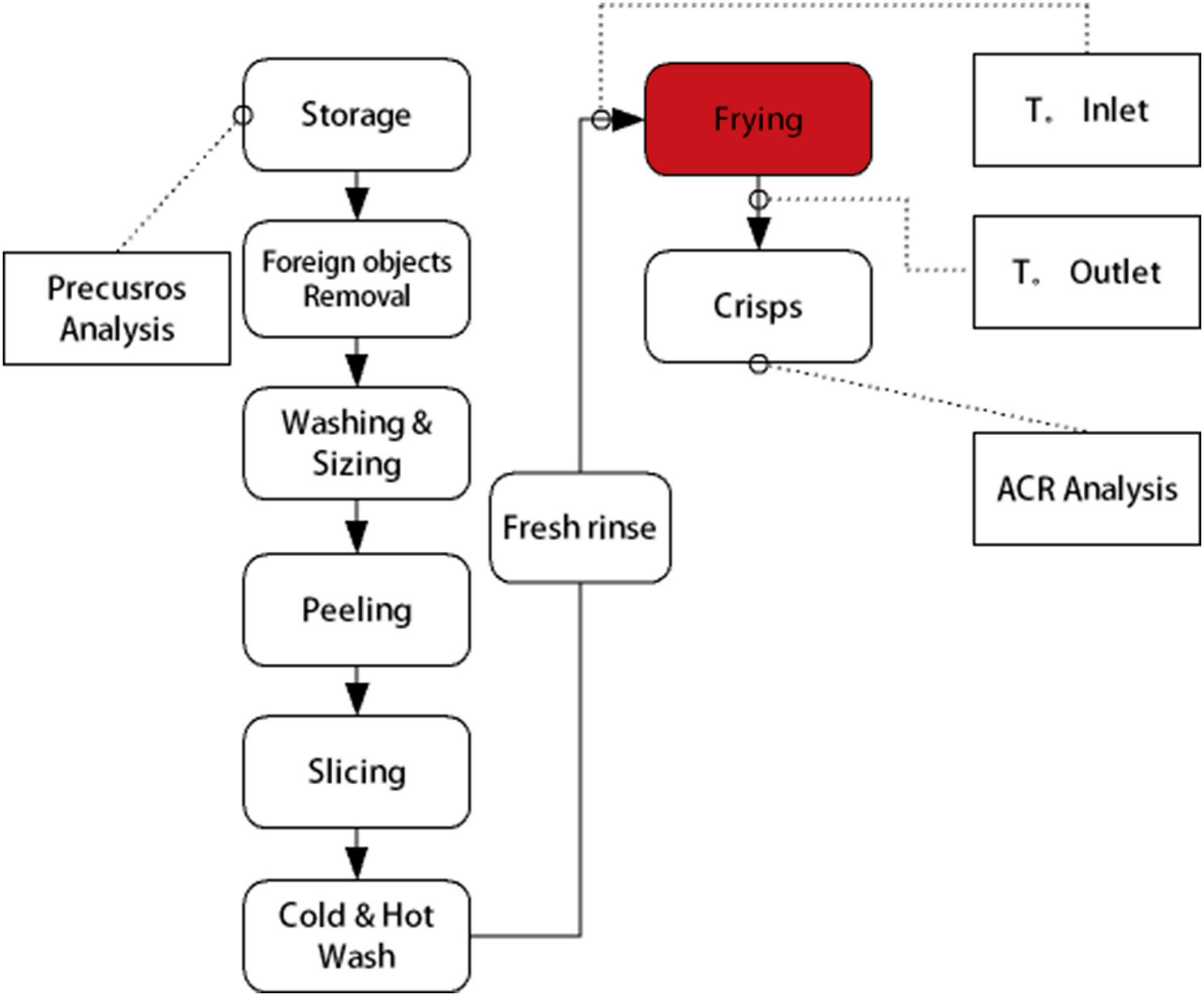
Figure 5 – Parallel coordinates analysis plot for 2017 / 2018 data

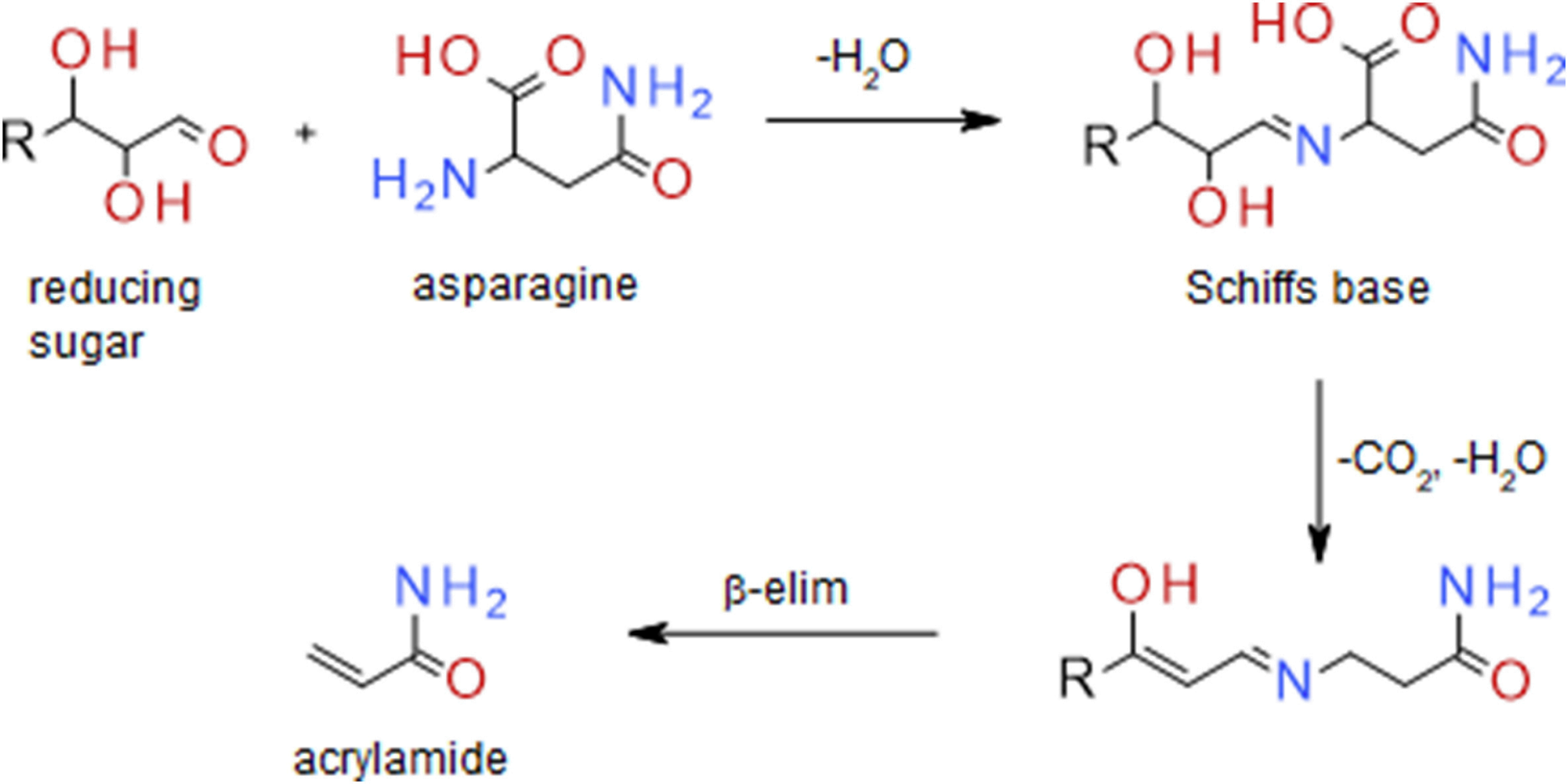
Figure 6 – Scores plot considering whether higher level ACR is differentiable. PC1 against PC2 for class 1 (< 750ppb acrylamide), and class 2 (>750ppb acrylamide).

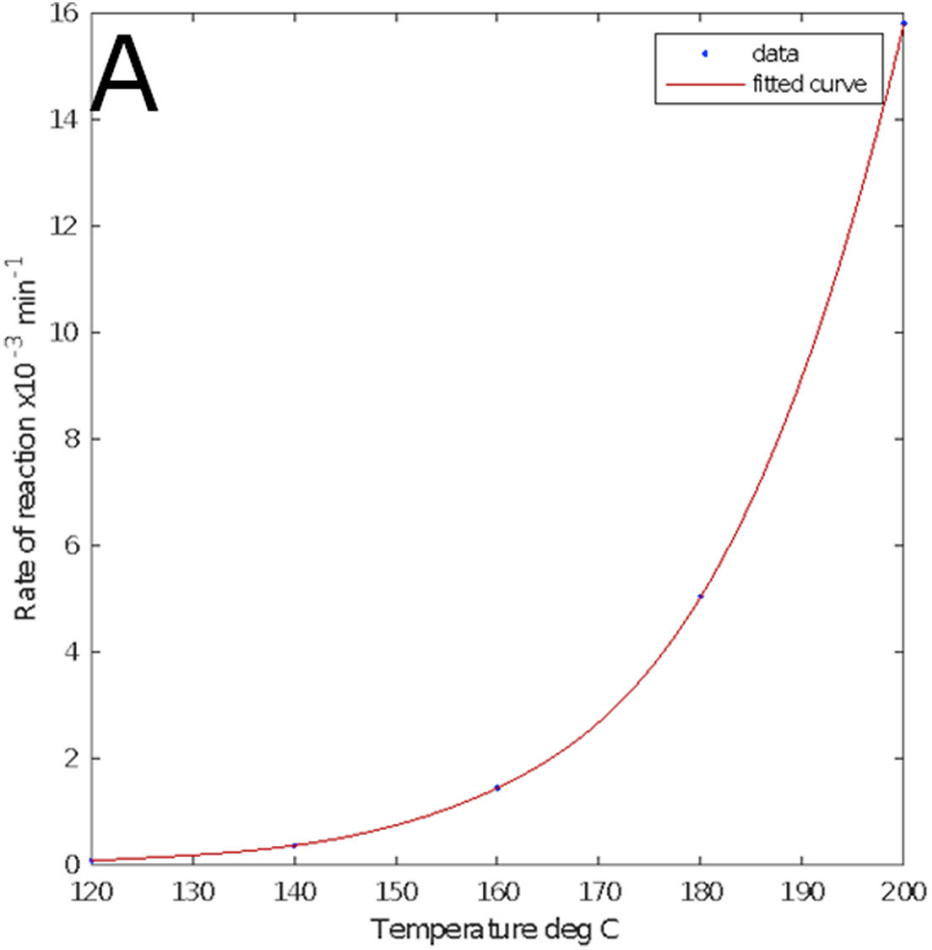
Figure 7 – Panel A: Probability of class 2 (>750ppb high acrylamide) prediction for training set (circles) and test set (stars). Panel B: Coefficients in PLS DA model for high acrylamide samples indicating extent of process variable contribution

Table 1 – Konelab accuracy

Table 2 – Analysis of misclassifications for varying the PLS DA probability threshold


Storage
Foreign objects Removal
Washing & Sizing
Peeling
Slicing
Cold & Hot Wash
Fresh rinse
Frying
Crisps
Precusros Analysis
T. Inlet
T. Outlet
ACR Analysis


OH
R
O
OH
HO
O
NH2
H2N
O
-H2O
OH
HO
O
NH2
R
N
O
OH
reducing sugar
asparagine
Schiffs base
-CO2, -H2O
β-elim
NH2
O
OH
NH2
R
N
O
acrylamide


A
data
fitted curve
Rate of reaction x10 -3 min-1
Temperature deg C
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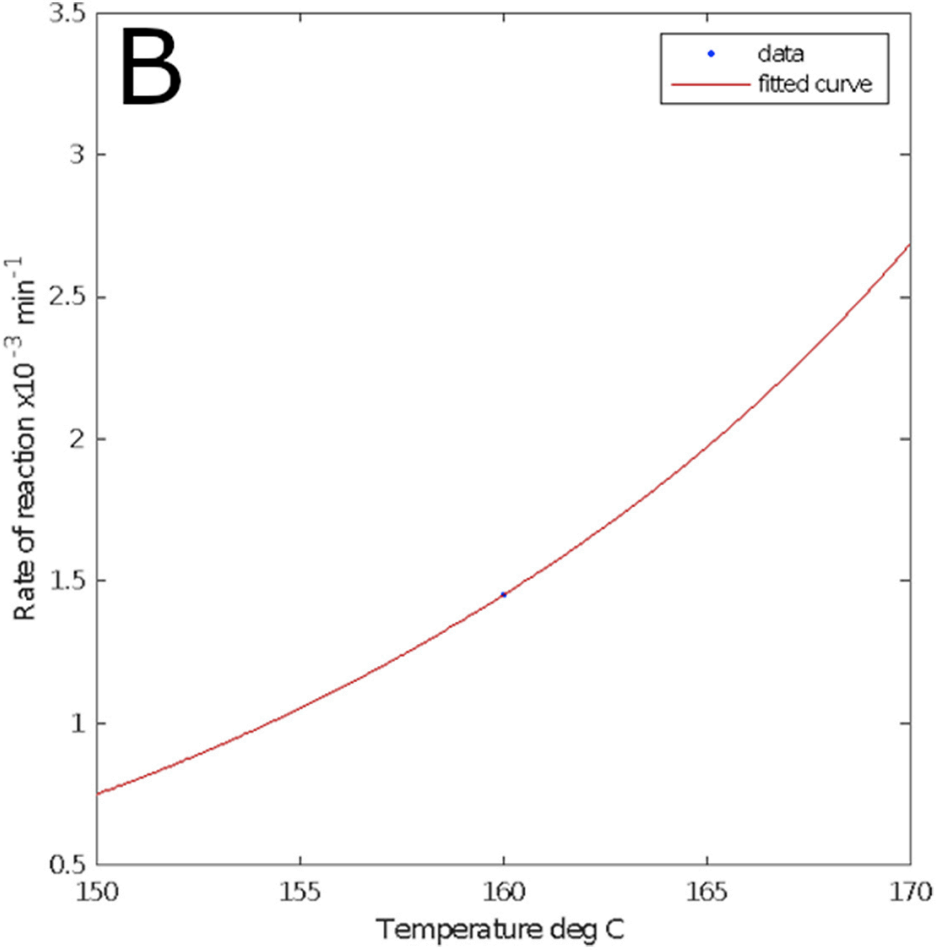
4
6
8
10
12
14
16
120
130
140
150
160
170
180
190
200


B
data
fitted curve
Rate of reaction x10 -3 min-1
Temperature deg C
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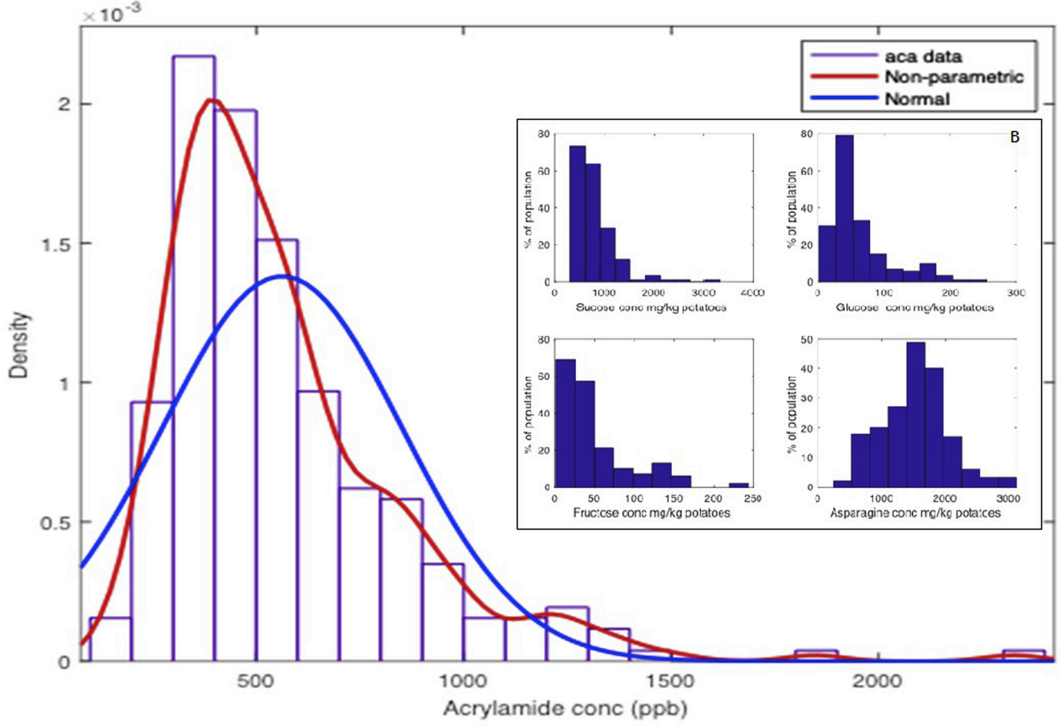
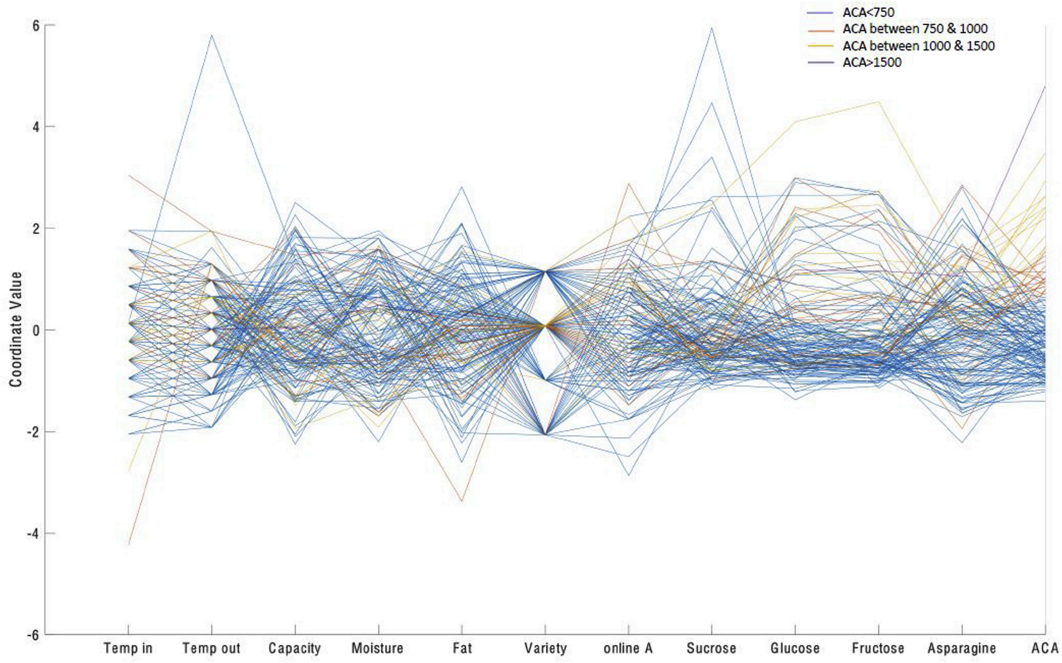
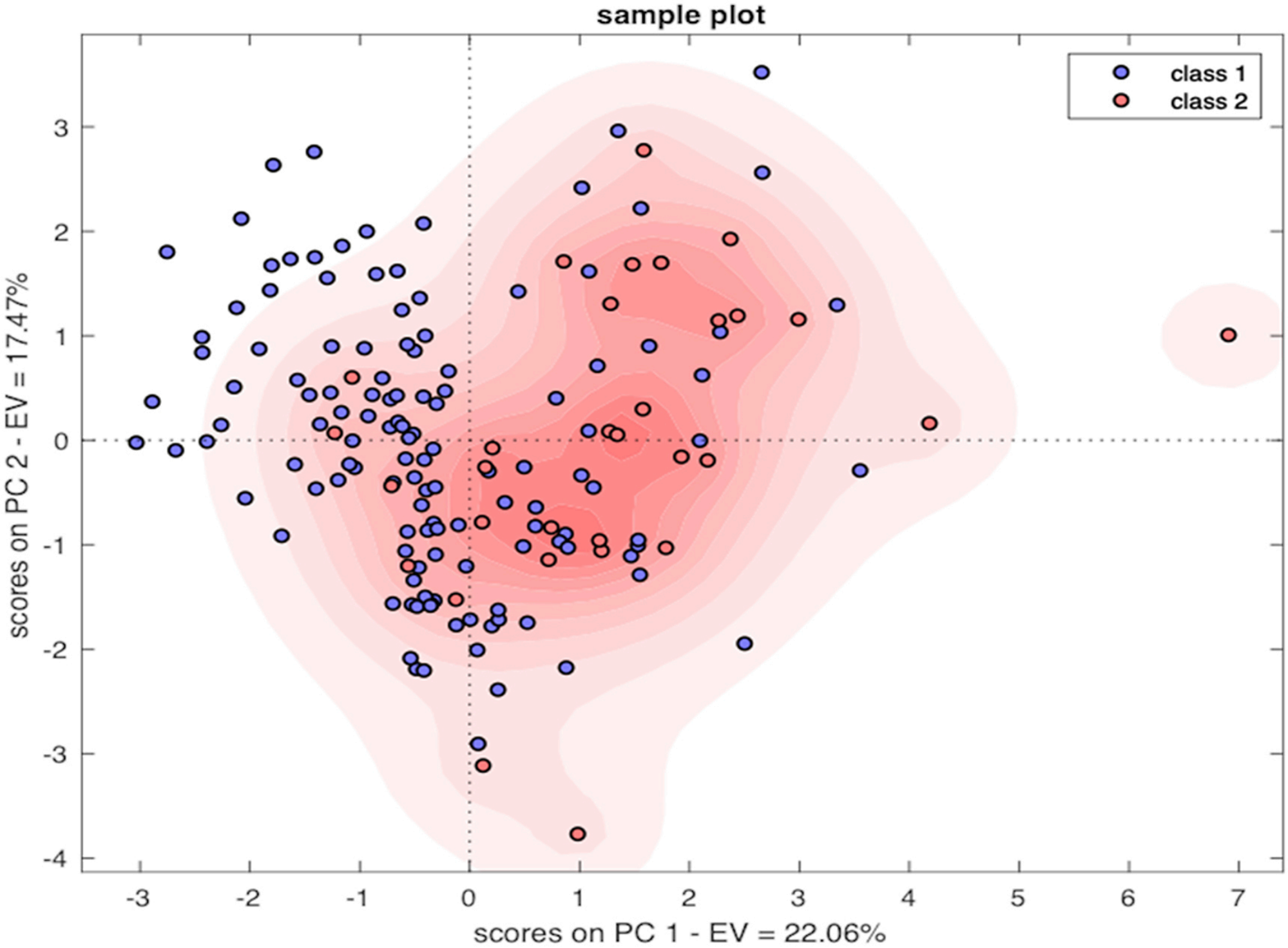
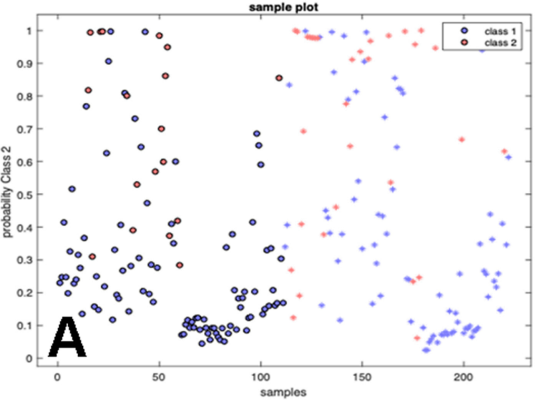
1
1.5
2
2.5
3
3.5
150
155
160
165
170


×10^-3
aca data
Non-parametric
Normal
Density
Acrylamide conc (ppb)
B
% of population
Sucose conc mg/kg potatoes
Glucose conc mg/kg potatoes
Fructose conc mg/kg potatoes
Asparagine conc mg/kg potatoes


ACA<750
ACA between 750 & 1000
ACA between 1000 & 1500
ACA>1500
Coordinate Value
6
4
2
0
-2
-4
-6
Temp in
Temp out
Capacity
Moisture
Fat
Variety
online A
Sucrose
Glucose
Fructose
Asparagine
ACA


sample plot
class 1
class 2
scores on PC 2 - EV = 17.47%
scores on PC 1 - EV = 22.06%
3
2
1
0
-1
-2
-3
-4
-3
-2
-1
0
1
2
3
4
5
6
7


sample plot
class 1
class 2
probability Class 2
samples
A

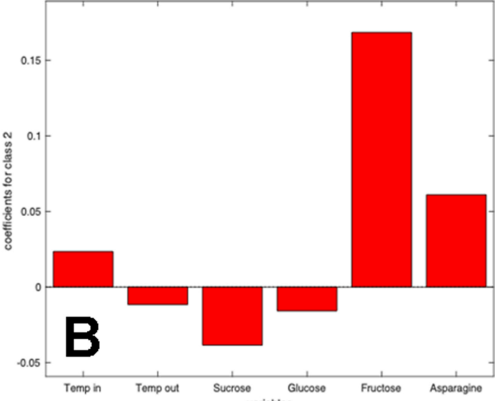

coefficients for class 2
Temp in
Temp out
Sucrose
Glucose
Fructose
Asparagine
variables
B

Table 1 - Konelab Accuracy

Precursor Name	**Avg. Confidence Boundary**
Fructose	± 0%
Asparagine	± 1.29%
Total Glucose	± 0.22%
Glucose	± 1.26%
Sucrose	± 0.15%

Table 2 – Analysis of misclassifications for varying the PLS DA probability threshold

Threshold at 0.75			**Threshold at 0.95**		
	Predict Low	Predict High		Predict Low	Predict High
Actual Low	58%	13%	Actual Low	64%	7%
Actual High	14%	15%	Actual High	18%	11%

Highlights

- **PLS on potato precursors has been applied to predict acrylamide formation within a factory setting**
- **The same approach to develop a prediction tool could be applied to other factories**
- **Approach allows food sector to monitor raw material suitability prior to processing**

Author Contribution Statement - **LWT-D-19-03587R1**

Moira Ledbetter: Investigation, Formal Analysis, Data Curation, Writing- Reviewing and Editing; **Leanne Bartlett**: Investigation, Formal Analysis, Data Curation, Writing- Original Draft; **Keith Sturrock**: Conceptualisation, Methodology, Supervision, Writing- Reviewing and Editing. **Alberto Fiore**: Conceptualisation, Methodology, Supervision, Project Administration, Visualisation, Data Curation, Writing- Reviewing and Editing. **Gary Montague**: Investigation, Formal Analysis, Data Curation, Writing- Original Draft; **Ged McNamara**: Investigation, Supervision, Data Curation, Writing- Reviewing and Editing.