



# Detection of multiple adulterants in tomato paste using near infrared spectroscopy

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# INTRODUCTION

Tomato concentrate is one of the best-selling tomato-based products.

Economically motivated food adulteration (EMA) problems arise frequently due to increasing market demands.

## Common tomato paste adulteration methods

- Wrong origin or ecological classification
- Unauthorized preservatives, acidity regulators
- Water, processing by-products, cheaper fillers → to dilute
- Starch, starch derivatives → to improve the rheological properties
- Sugar, salt → to increase the soluble solid content
- Extracts, dyes (Sudan dyes) → color adjustment

The complex nature of some adulterants can outmaneuver detection with conventional methods



# AIM OF THE RESEARCH

We examined tomato concentrates.

The study aims to apply **NRS** and **aquaphotonics** to detect and predict low concentrations of ground paprika seed, sugar and salt in tomato concentrates.



# MATERIALS

Ground paprika seed



Sugar - sucrose



Salt - NaCl



Corn starch



- + water\*
- |    |      |
|----|------|
| 1. | 0,5% |
| 2. | 1%   |
| 3. | 2%   |
| 4. | 5%   |
| 5. | 10%  |

- |    |      |
|----|------|
| 1. | 0,5% |
| 2. | 1%   |
| 3. | 2%   |
| 4. | 5%   |

\*Water in specific concentration

Potential combinations: T, C, S, WP, CS, WPC, WPS, WPCS

30 different compositions samples, preparation in triplicate → 90 samples

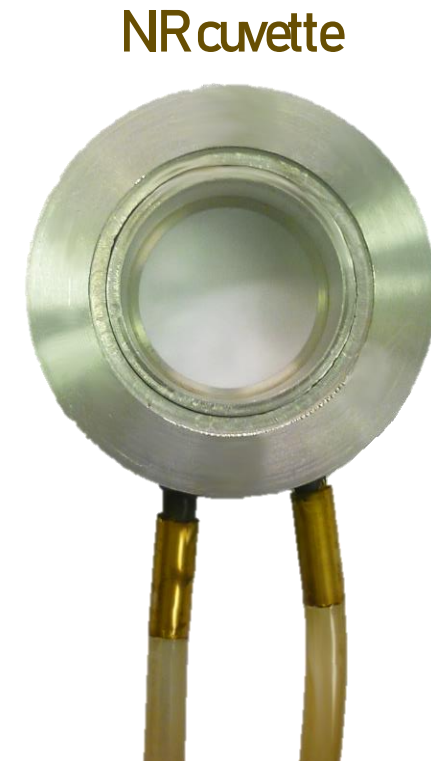
# METHODS

## Near infrared spectroscopy – NRS

Measuring instrument: MetriNR benchtop NR spectrometer

Measuring conditions:

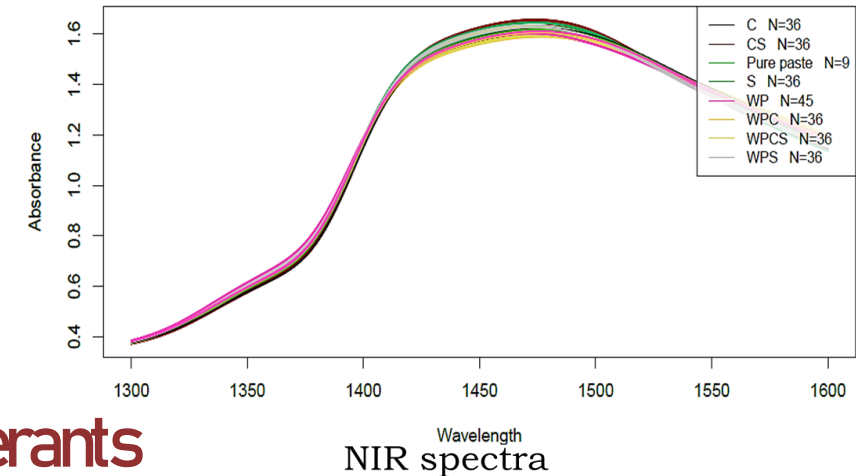
- Thermoregulated cuvette, 25°C
- Layer thickness: 0.4 mm
- Spectral range: 740 – 1700 nm
- Randomized measurement sequence
- 3 consecutive scans per sample



# STATISTICAL METHODS

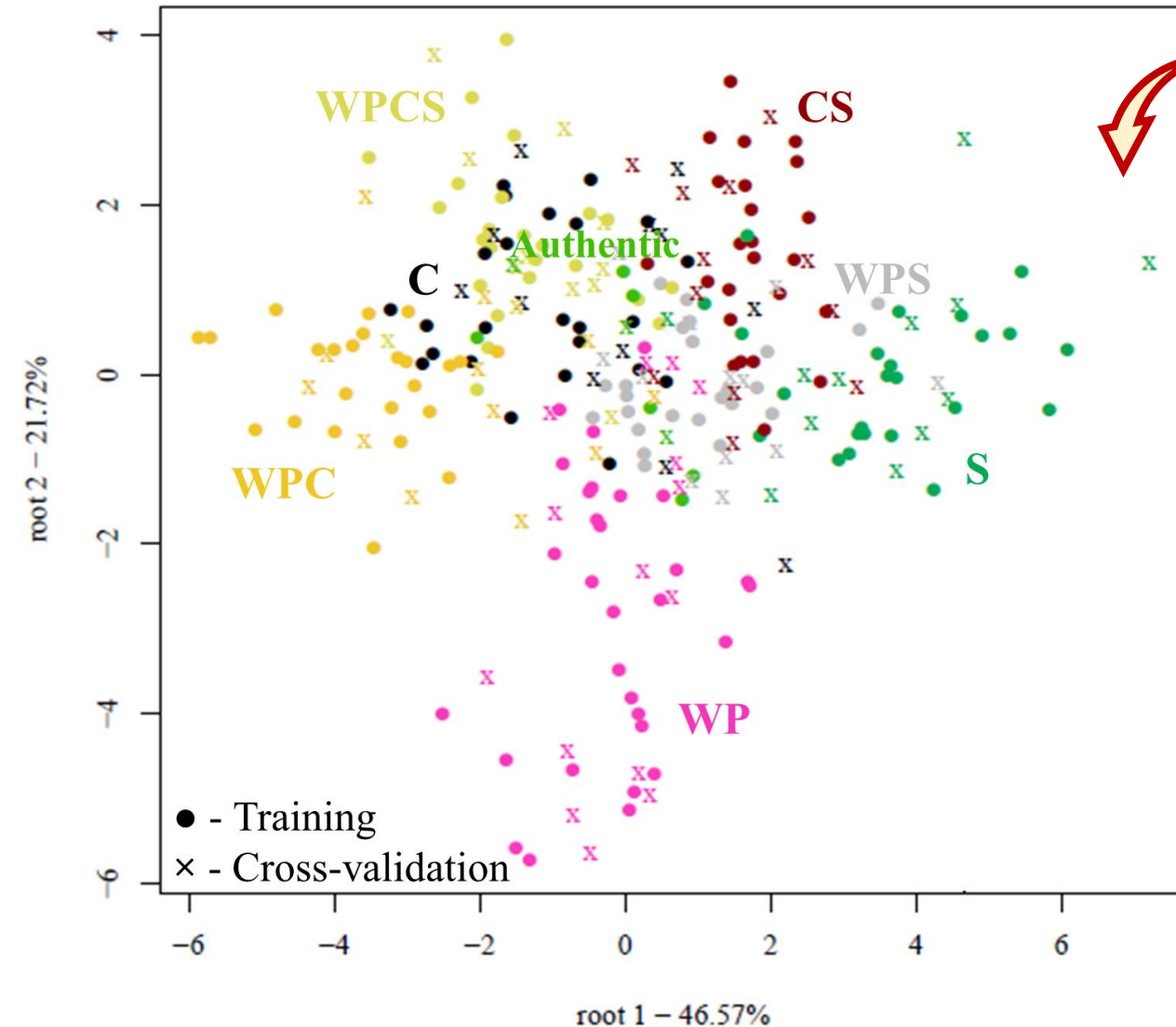
## Multivariate analysis

- **Pretreatment of raw data**
  - ✓ 1300 – 1600 nm wavelength range
  - ✓ Savitzky-Golay smoothing filter - 2<sup>nd</sup> order polynomial
  - ✓ Multiplicative scatter correction – MSC
- **Linear discriminant analysis – LDA** – to classify adulterants
  - ✓ Three-fold cross-validation
- **Partial least squares regression – PLSR** – to predict adulterant concentration
  - ✓ Validation by „Leave one sample out”
- **Aquagram** – to visualize changes in spectral patterns



# RESULTS – LDA

## Discrimination of different adulterations in tomato pastes



### All adulteration:

- Recognition: 91.11%
- Prediction: 57.99%

### Samples containing paprika seed

- Recognition: 98.89%
- Prediction: 65.46%

### Prediction of concentrations

#### Simple adulterations

- Paprika seed: 77.74%
- Sugar: 71.35%
- Salt: 95.32%
- Water: 77.74%

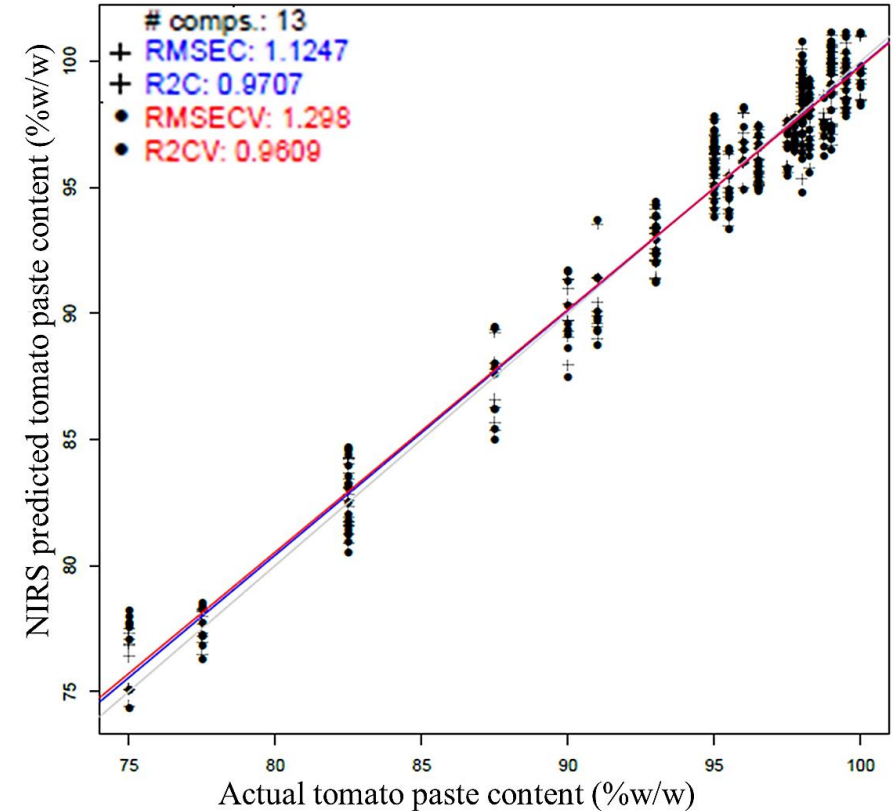
# RESULTS – PLSR models to predict adulterant concentration

## Samples with simple adulteration

| <i>Adulterant</i> | $R_c^2$ | RMSEC (%w/w) | $R_{cv}^2$ | RMSECV (%w/w) |
|-------------------|---------|--------------|------------|---------------|
| Paprika seed      | 0.947   | 0.526        | 0.935      | 0.584         |
| Sugar             | 0.933   | 0.429        | 0.918      | 0.475         |
| Salt              | 0.982   | 0.224        | 0.978      | 0.248         |
| Water             | 0.947   | 0.789        | 0.935      | 0.875         |
| Tomato paste      | 0.971   | 1.125        | 0.961      | 1.298         |

$R^2$  – coefficient of determination

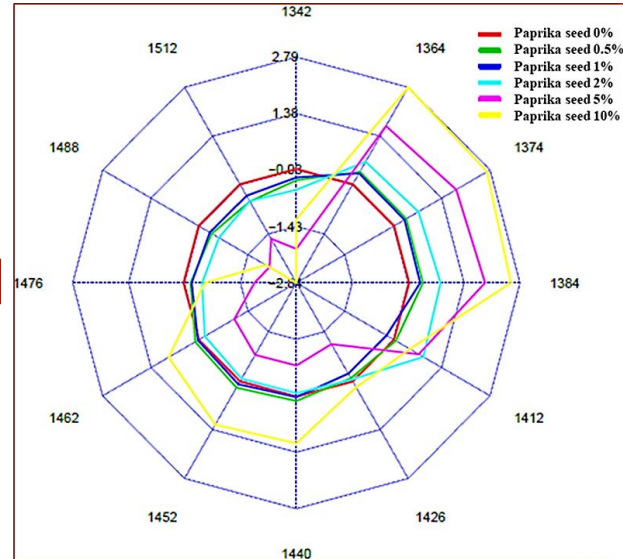
RMSE – root mean square error



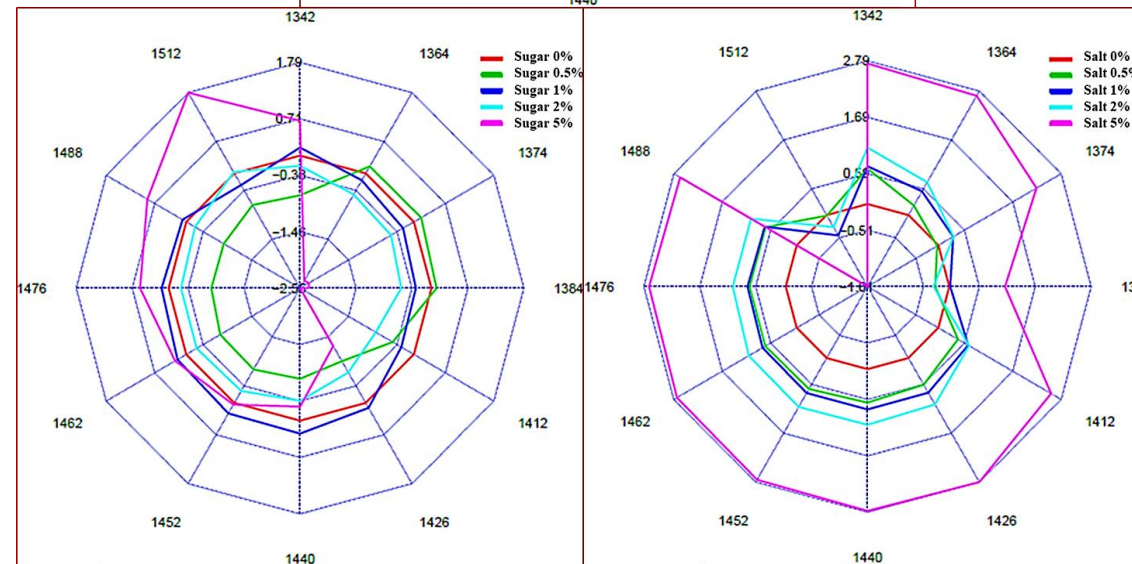
# RESULTS – Aquagrams

## Samples with simple adulteration

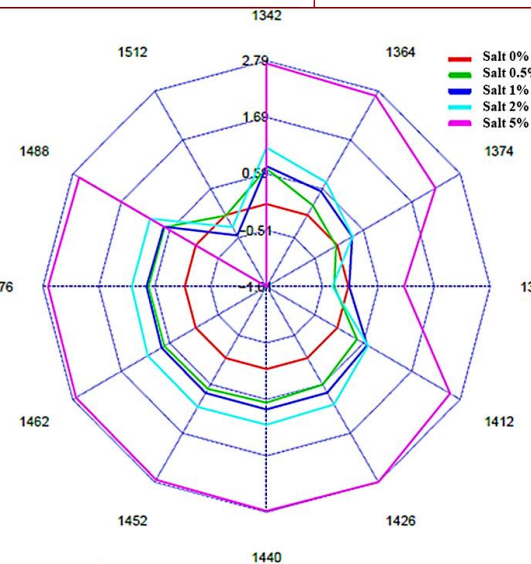
Ground paprika seed



Sugar



Salt



```
# AQUAPHOTOMICS POSTER PRESENTATION END
col = DAdat$col$C_type
pdf("Results/Aquaphotomics_PosterFlash_END.pdf")
TranInd = -seq(1, nrow(DAdat), 3)
DA1 <- FDA_PCModels(DAdat, "C_type", NrPCs = 1:60,
                    TranInd= TranInd)
plotFDAModel(DA1, projCVres = TRUE,col = col[TranInd],
             col2 = col[-TranInd],

             main = „Thank You for your attention!“),
             legend("bottomright", legend= unique(DAdat$C_type),
                   col = unique(col), pch = 16, cex = 0.8)

write.xlsx(conftable,file = „Results/Poster.xlsx“,colNames=TRUE)

dev.off()
```