Joint selection of wavelength regions for mid-IR and Raman spectra and variables in PLS regression using Genetic Algorithms

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Université Montpellier 1 - France
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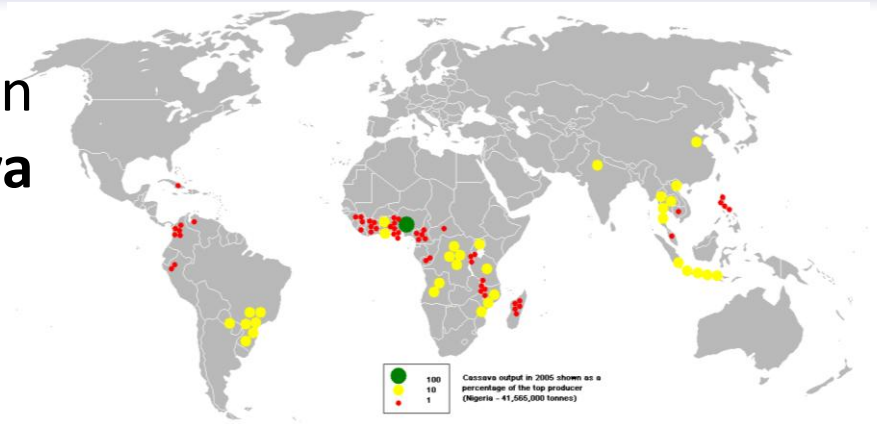
Université Montpellier 1 - France

The Context

Increased production and consumption of **cassava**



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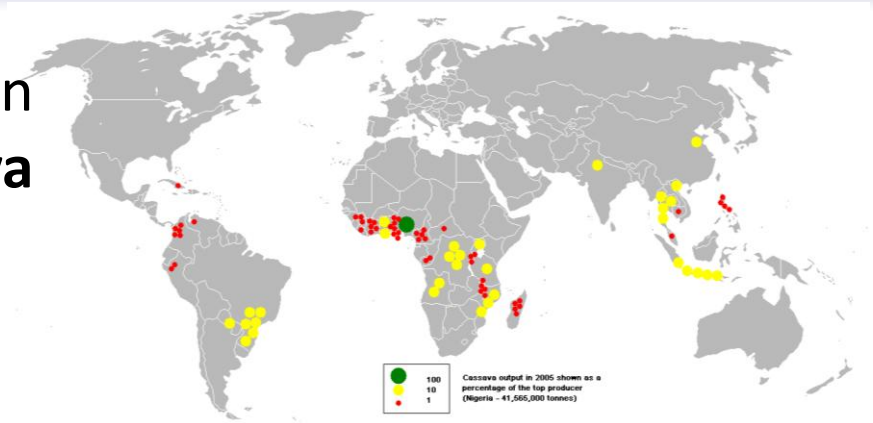

From the crop to the starch

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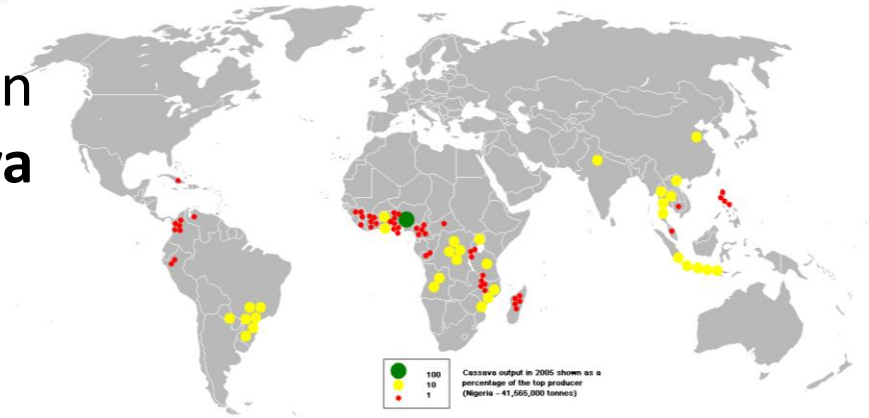

From the crop to the starch

Empirical and small-scale processing

Interest

Good breadmaking ability

The Aims

Physicochemical parameters

↓

Varietal and process impacts on breadmaking ability

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Physicochemical parameters

↓

Varietal and process impacts on breadmaking ability

Aim

✓Standardize and scale-up the process

✓Improve product quality

✓Industrial development of new gluten-free bread products

The Data

13 varieties x 4 treatments = 52 samples

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1. **Physicochemical parameters**

The Data

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1. Physicochemical parameters

Breadmaking ability

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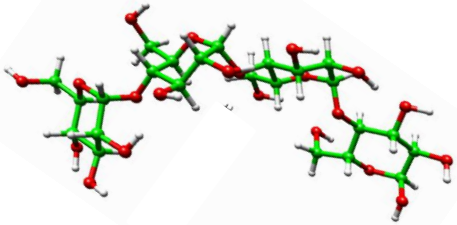
1. Physicochemical parameters

Breadmaking ability

Amylose content



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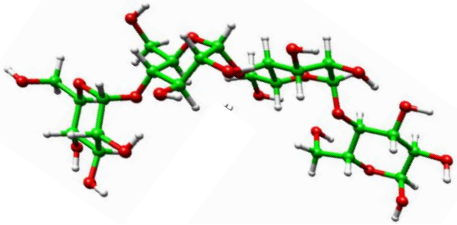
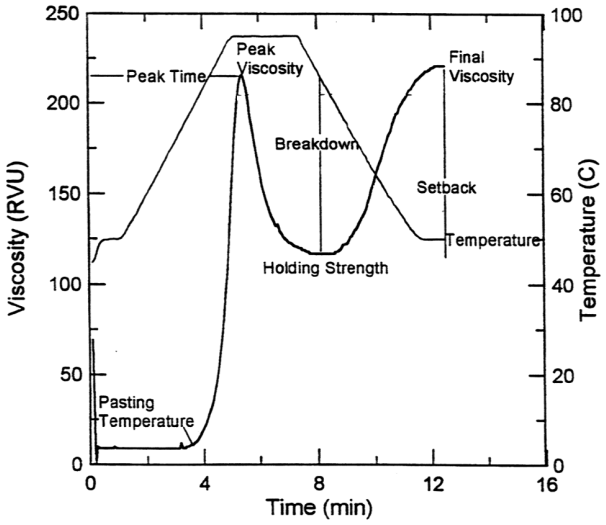


Rapid Visco Analyzer

Pasting behavior

12 variables



The Data

2. Spectral data

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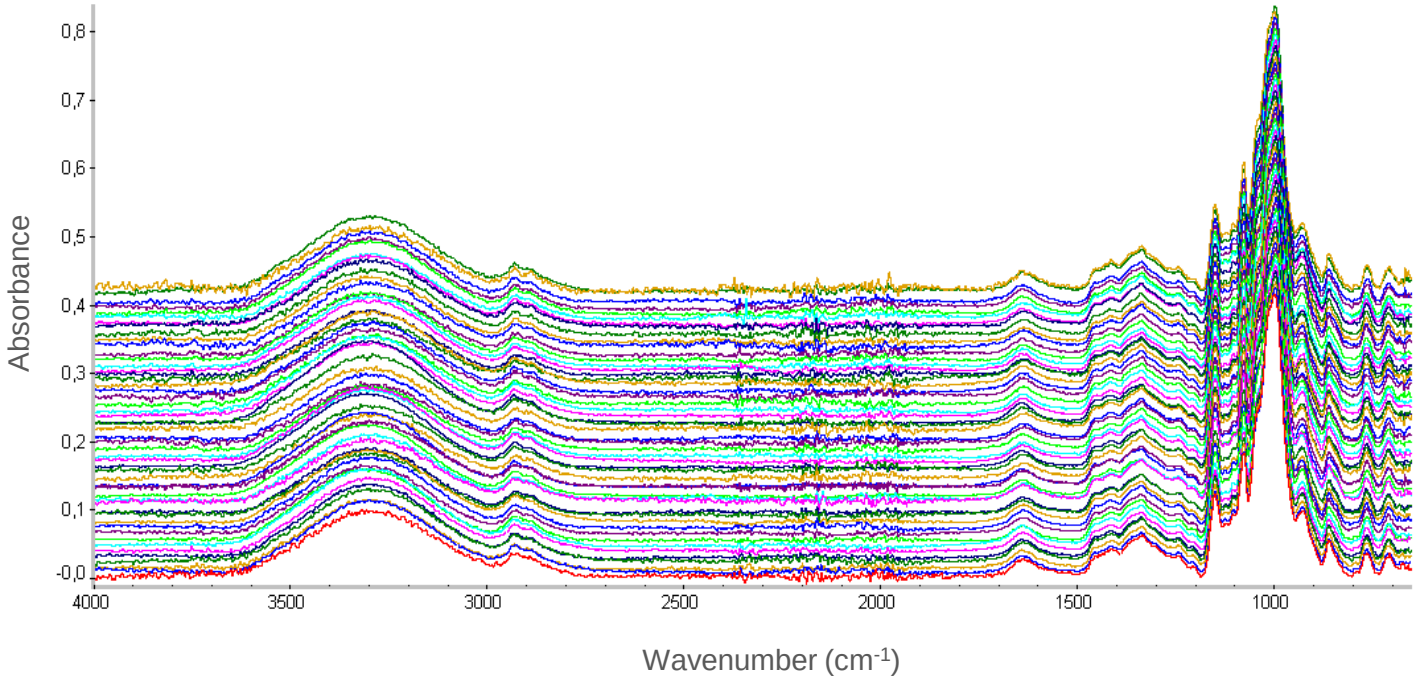
Mid-infrared spectra



650 – 4000 cm^{-1} ➡ 3351 variables

The Data

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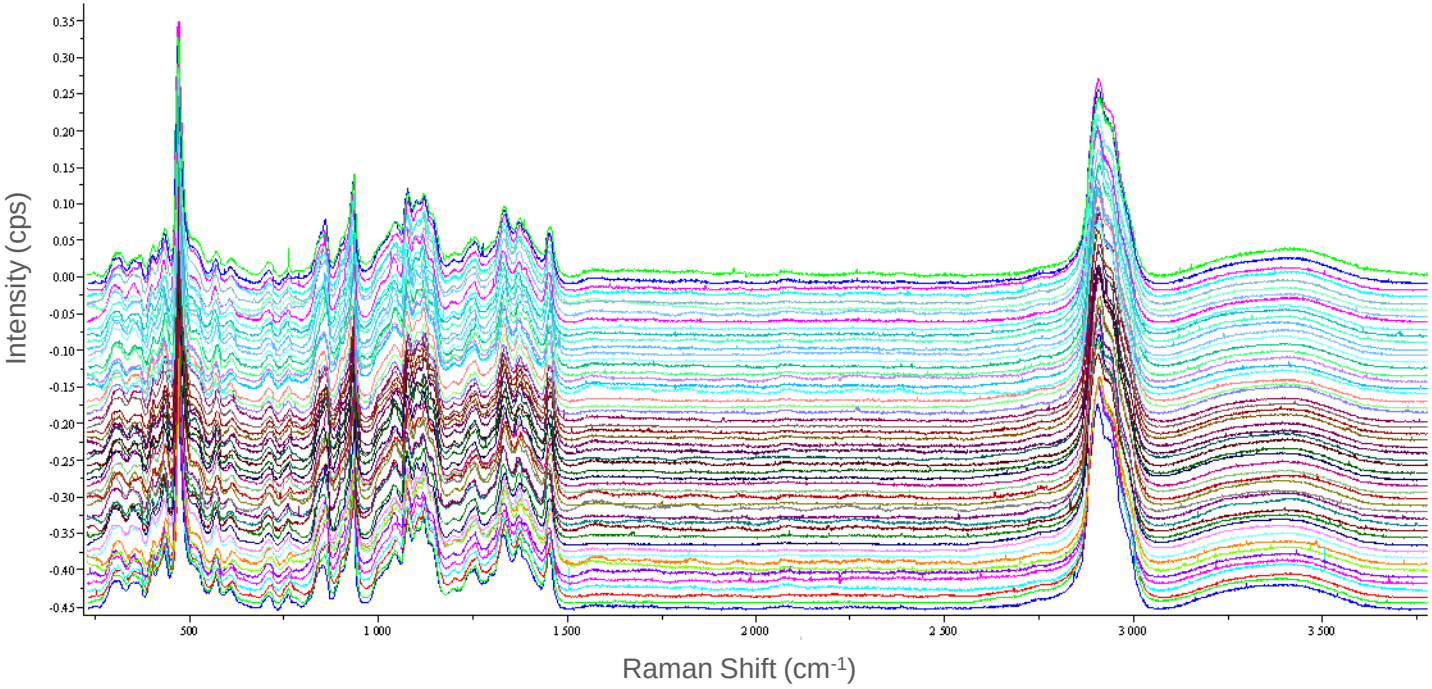
Raman spectra



230 – 3800 cm^{-1} ➡ 4562 variables

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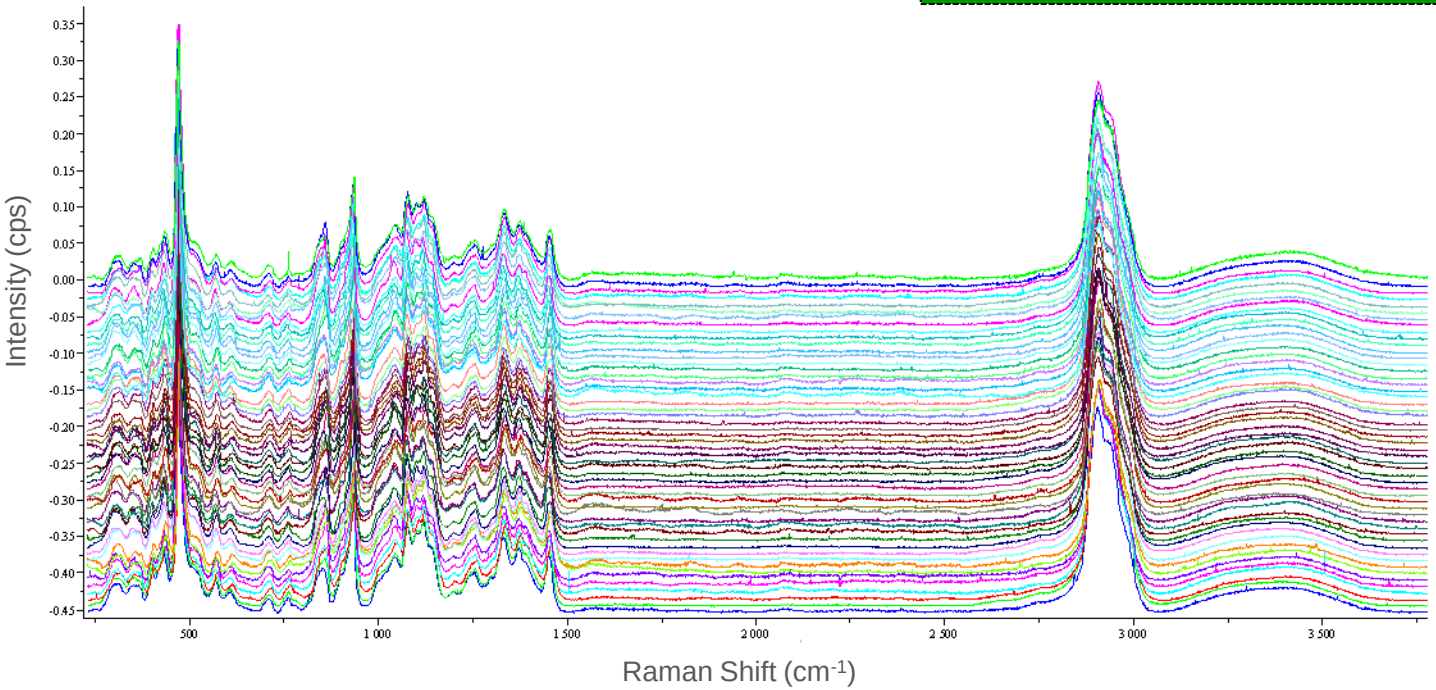
2. Spectral data

Raman spectra

Raman + IR
Pre-treatment
Baseline + SNV



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The Problematic

Data → **Predicting the expansion ability**

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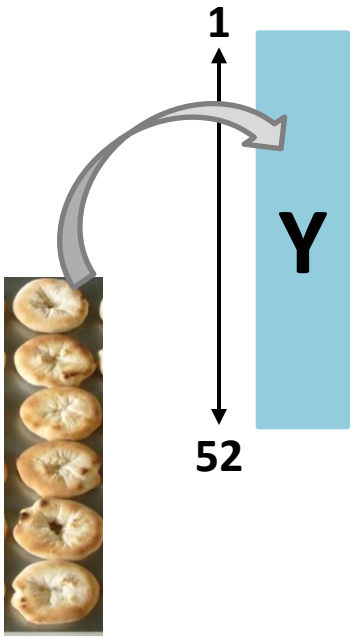

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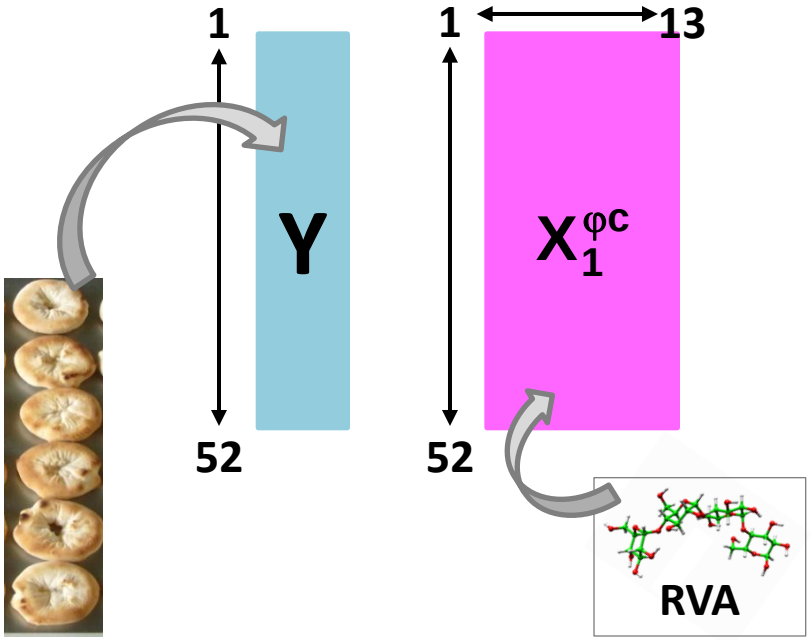

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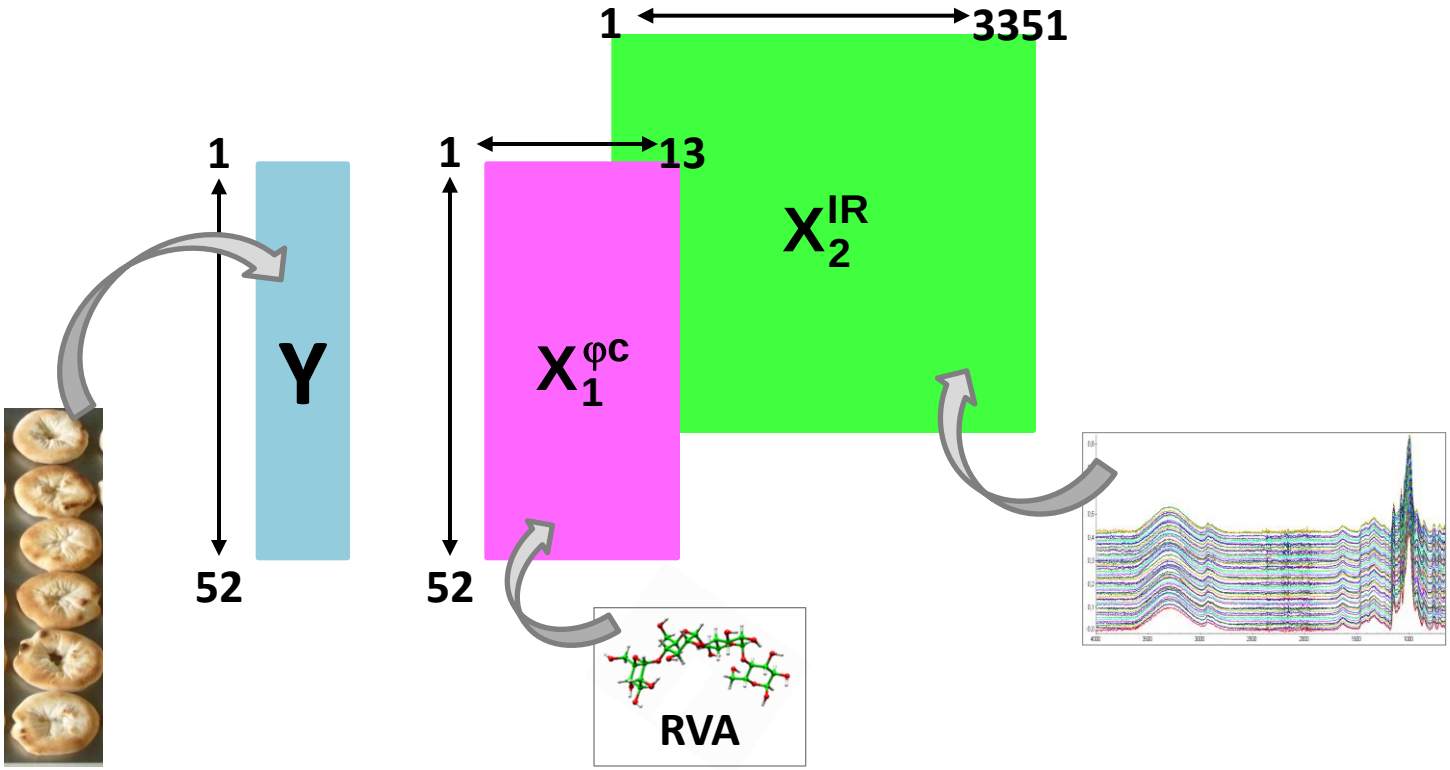

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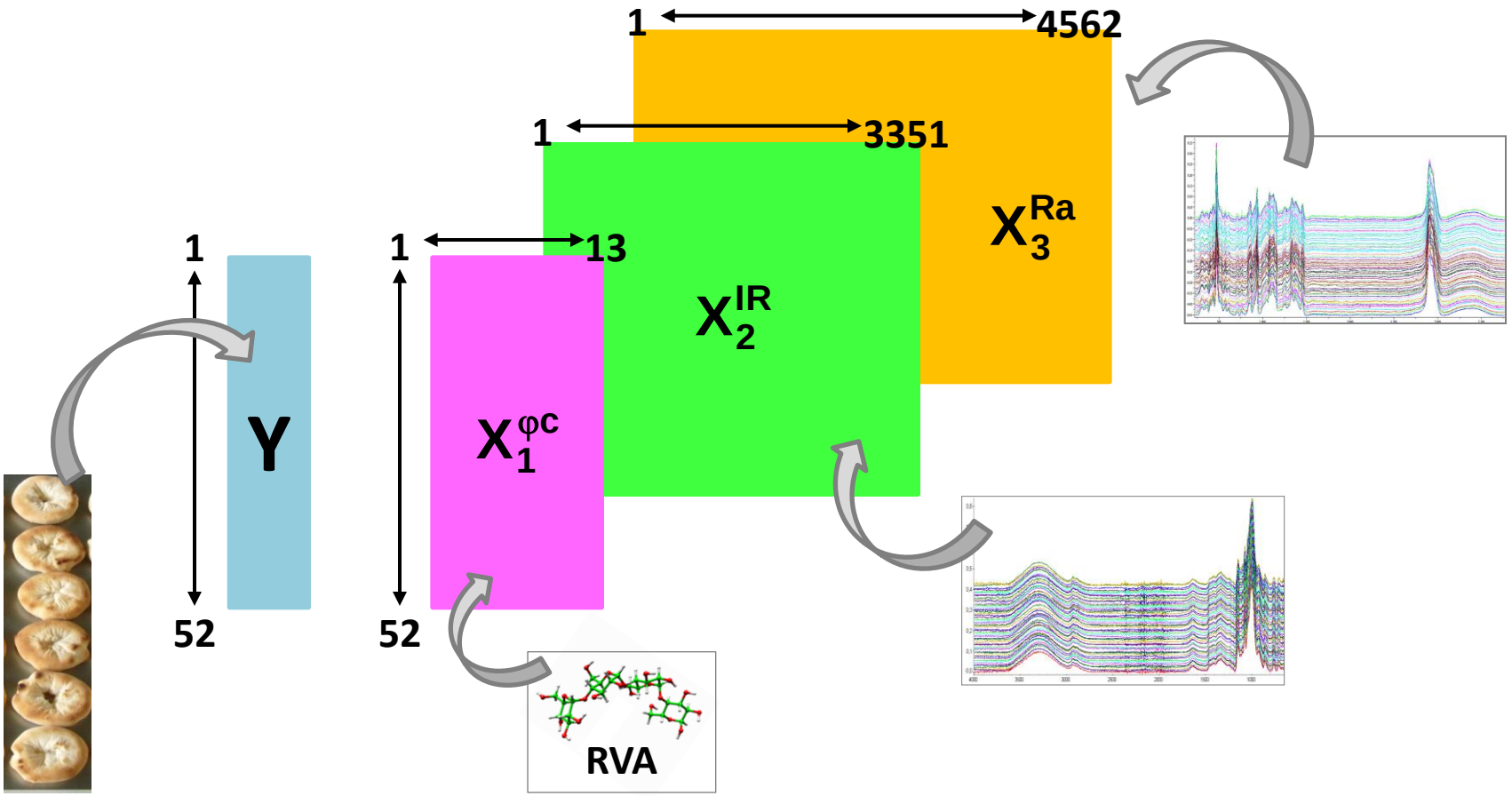

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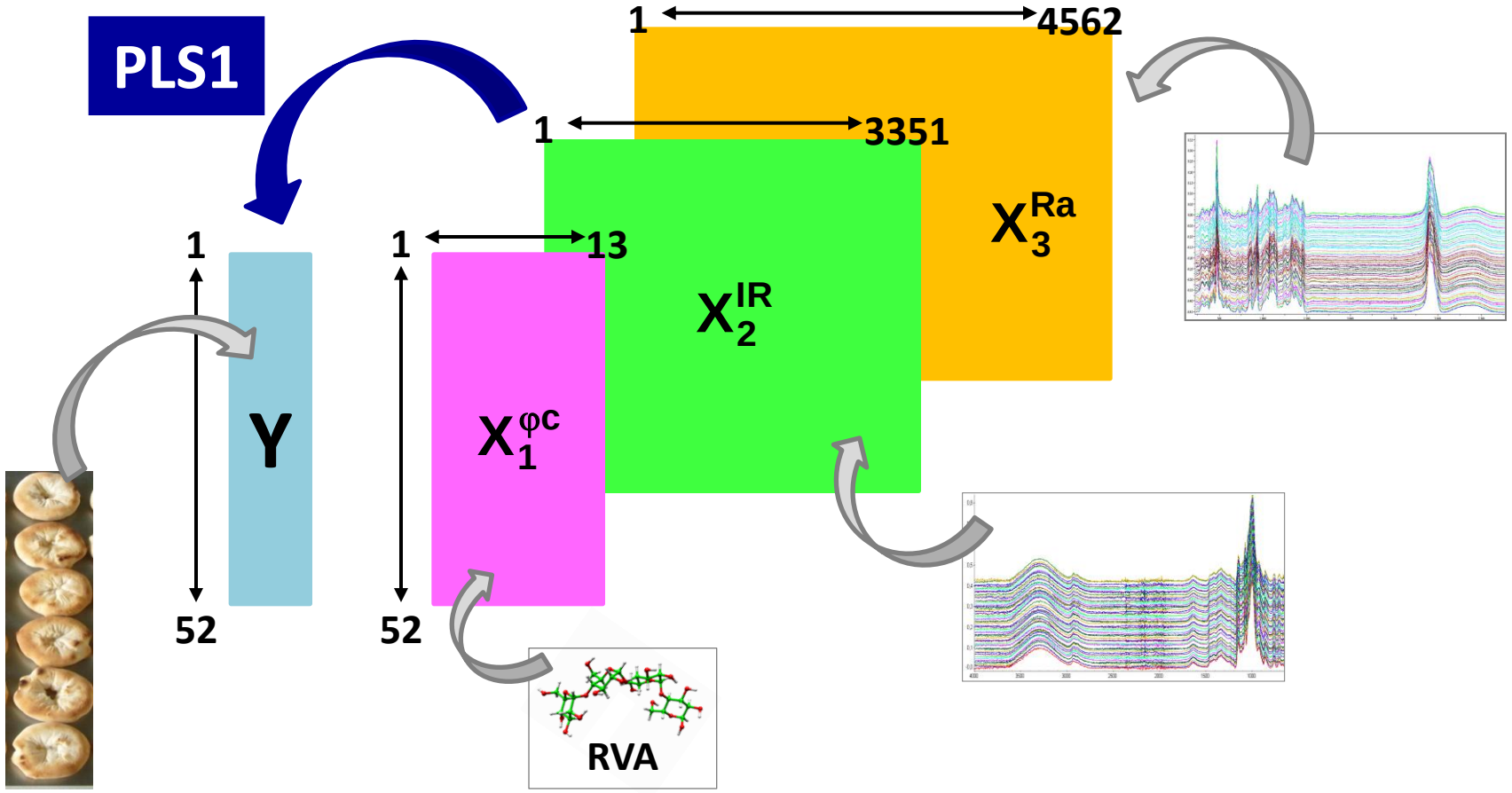

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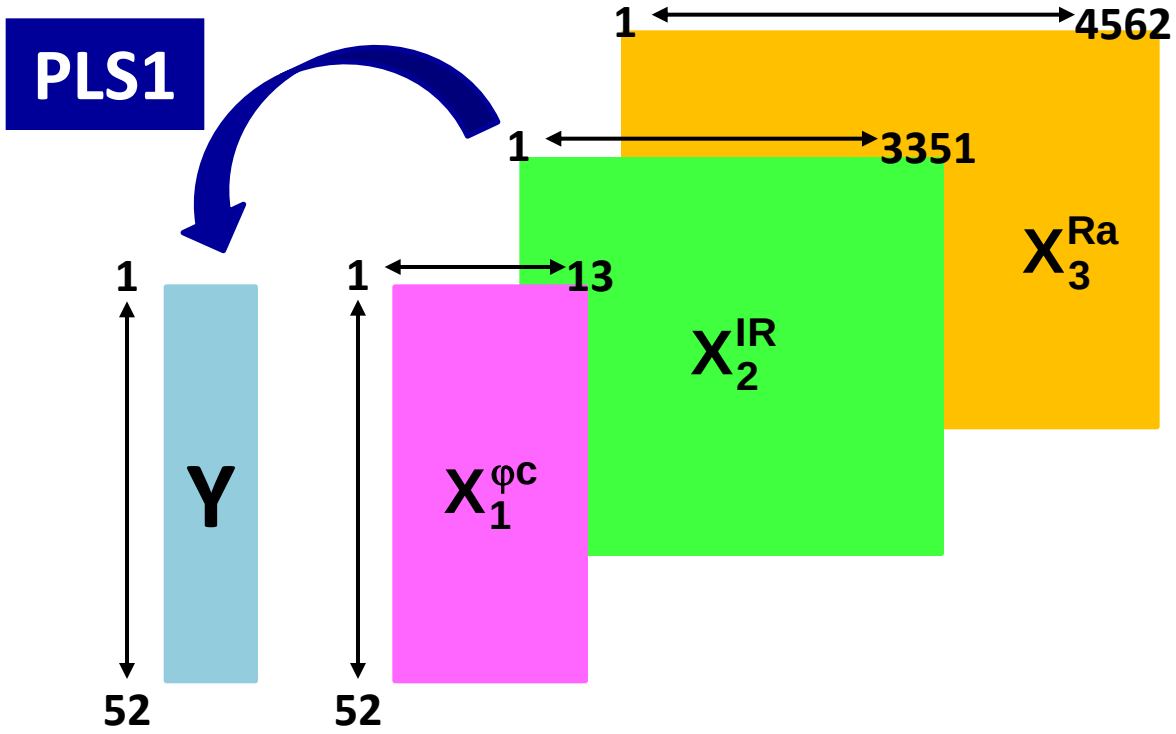

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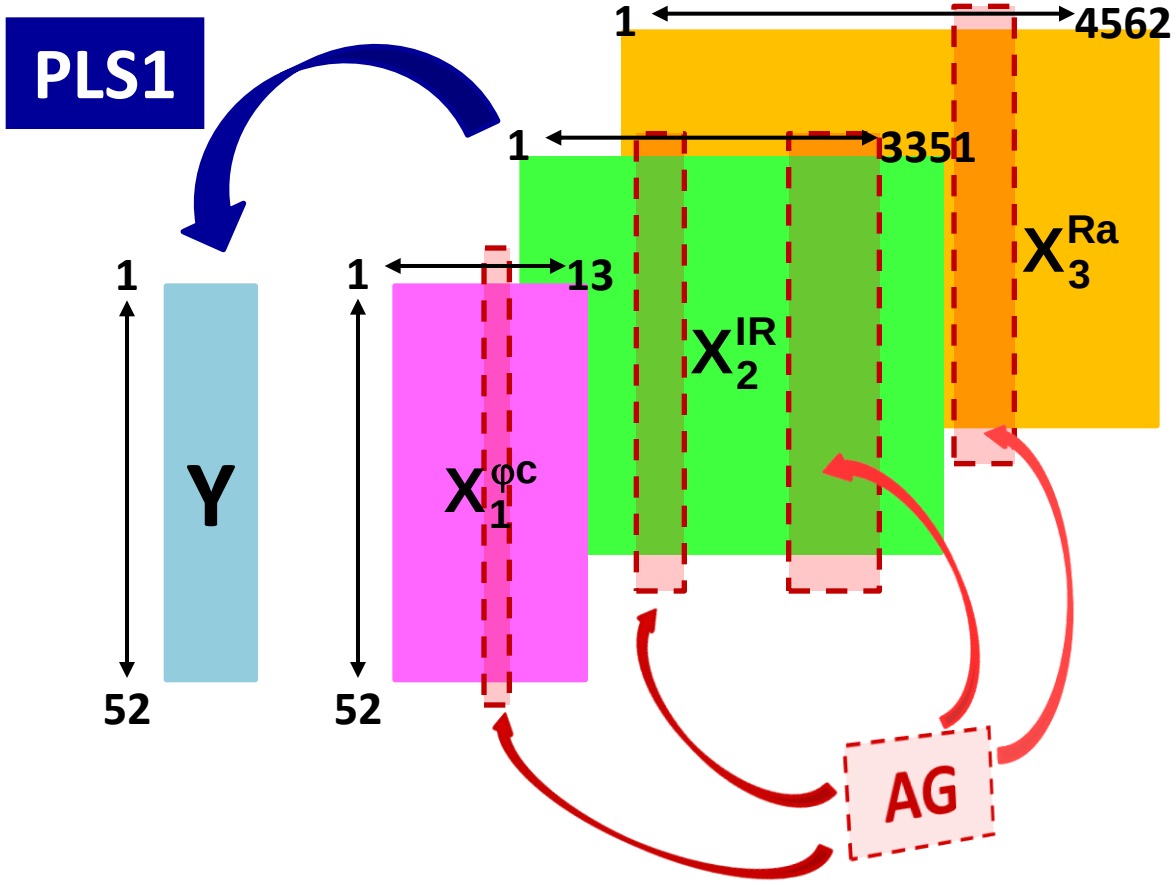

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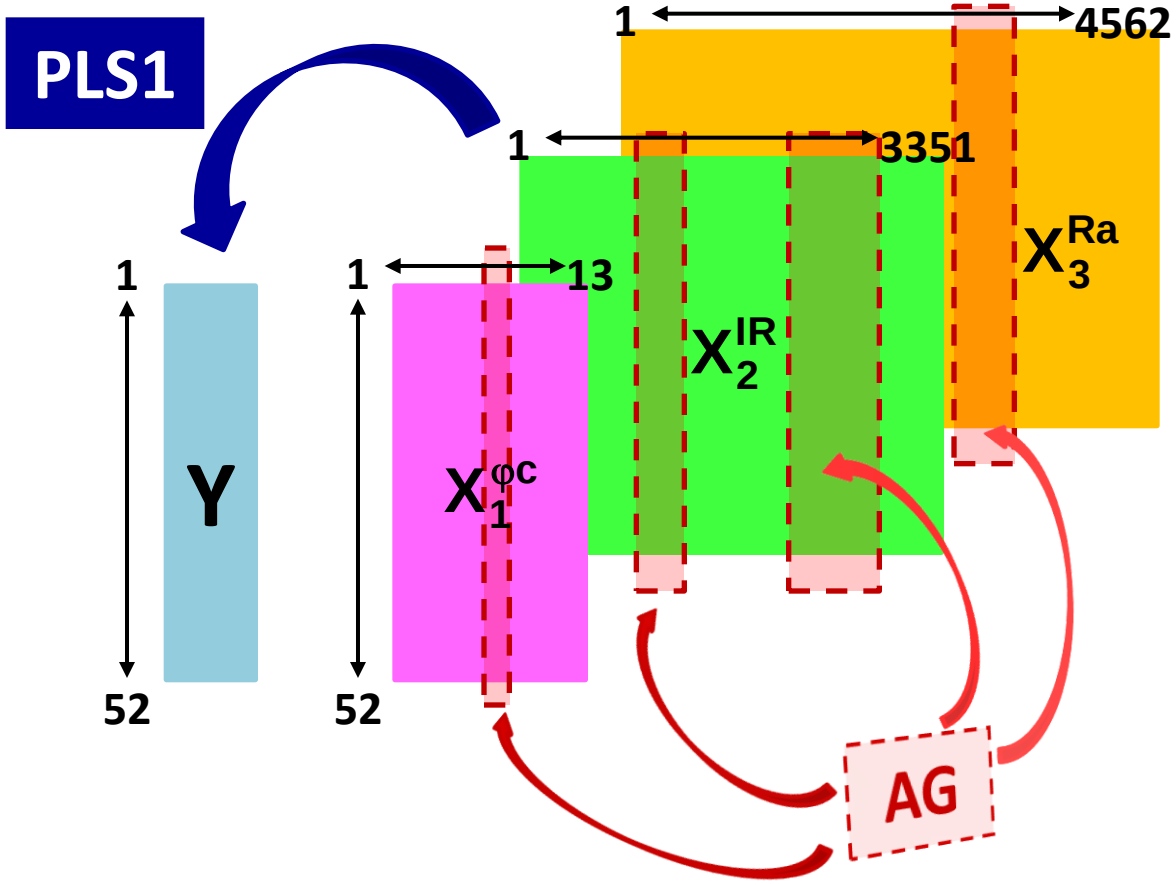

➡AGvPLSm

Genetic Algorithm

➡ optimization method based on the evolution of a « **population** » of potential solutions thanks to genetic mechanisms

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- crossover

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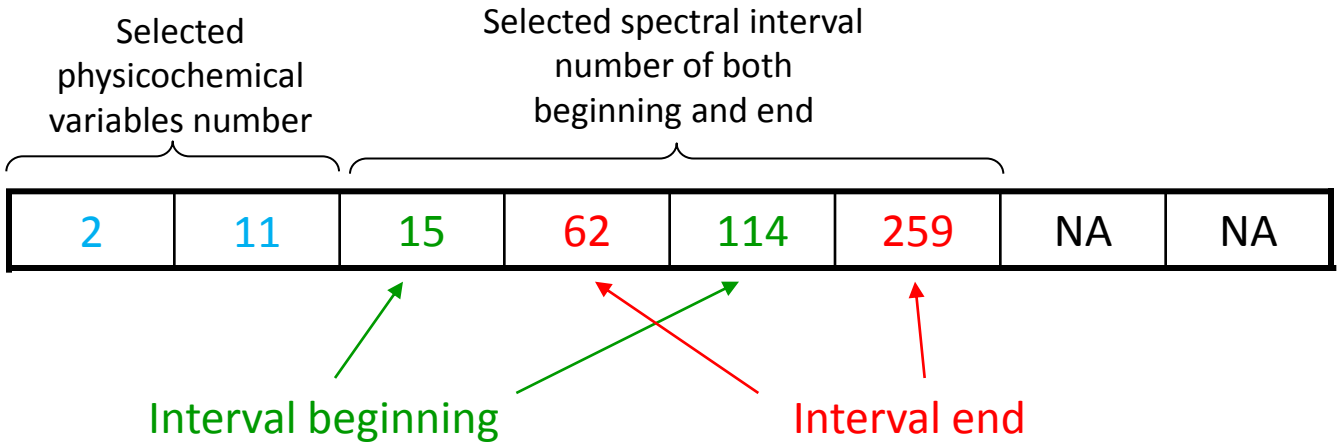
❸ Final population obtained after convergence criterion met

Genetic algorithm application to feature selection

One solution = a subset of variables (individual physicochemical variables + spectral intervals)

- **Individual encoding:**



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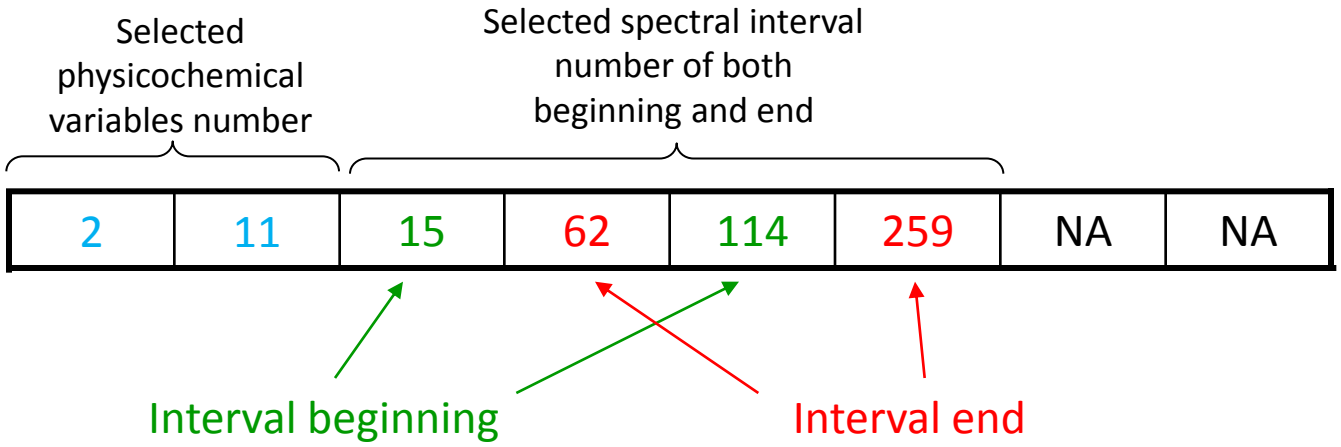

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  - Choice of the number of selected variables and/or interval between 1 and *Nmax*
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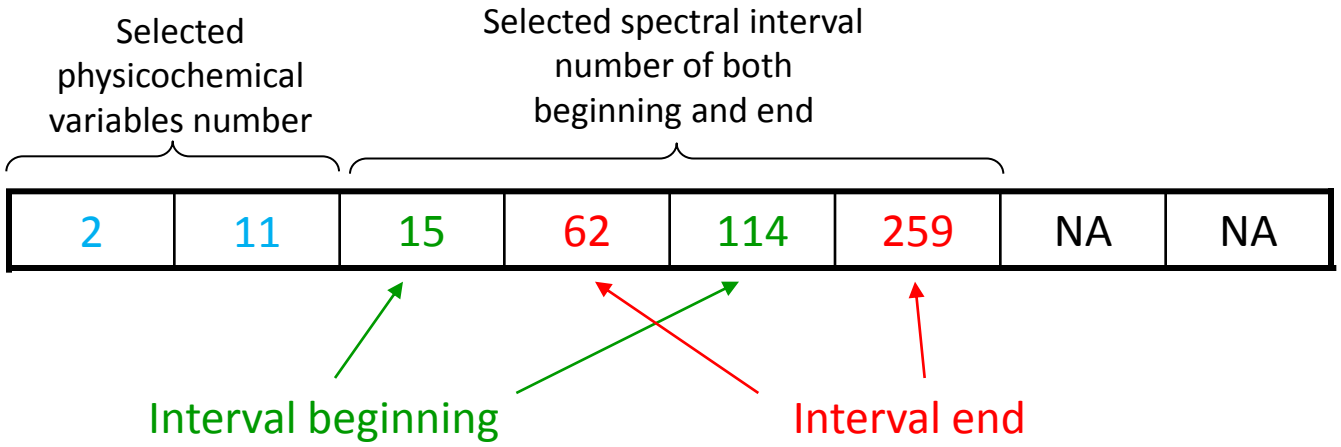

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physicochemical table → one variable

spectral tables → one interval

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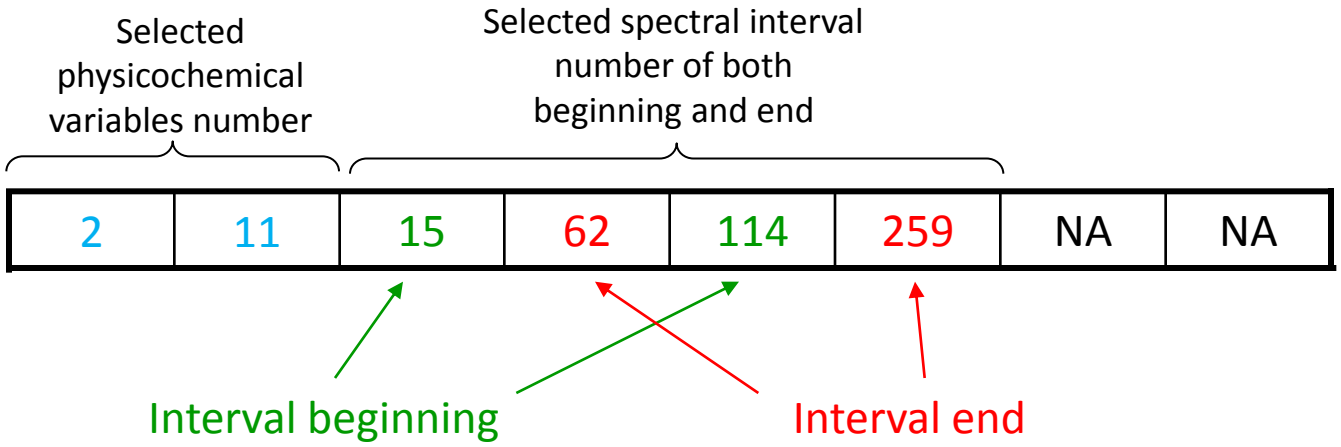

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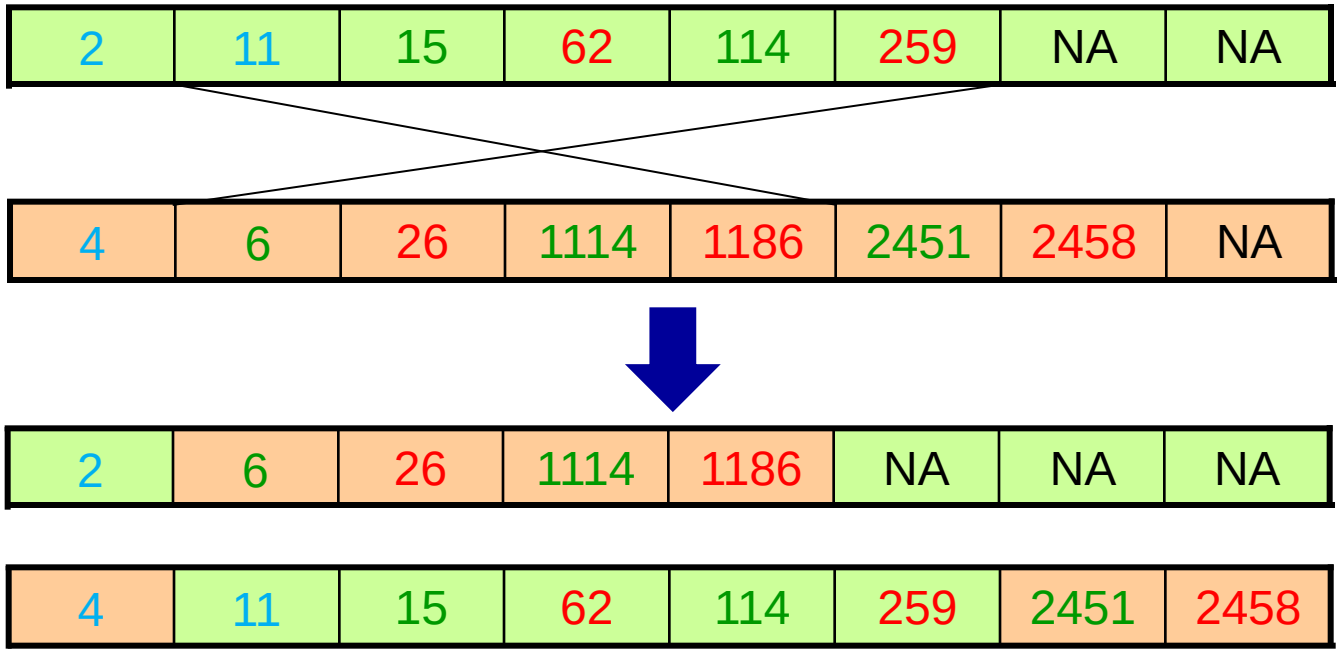
- **Crossover**: allows to combine characteristics of previously selected individuals



Genetic algorithm application to feature selection

- **Fitness function:** quantification of solution quality

$$fitness = \underbrace{R^2_{CV}\left(y, \hat{y}\right)}_{\text{Model precision}} + \underbrace{c \times \left(\alpha\left(N_{\text{varsel}} + \beta\right)\right)}_{\text{Model parsimony}}$$

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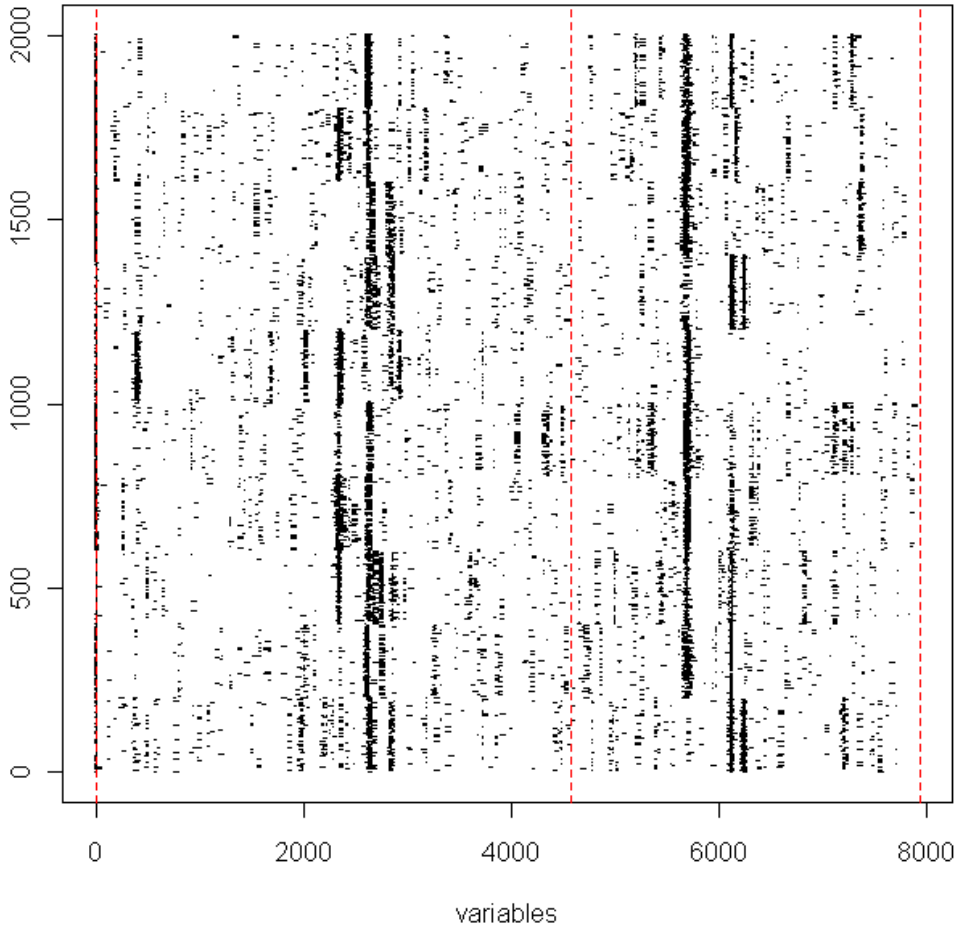
- **Selection operator:**
  - Ranking of solutions according to the fitness (the best one having the highest rank)
  - Compute selection probability for each solution : $p(\#k) = \gamma\, k + \nu$

    γ and ν are fixed so that the best solution selection probability is twice higher than the median solution one and the sum of all selection probabilities is one
  - Build a new population according to these probabilities with constant size

Results

GA results for 10 runs with population of size 200 and 100 generations:



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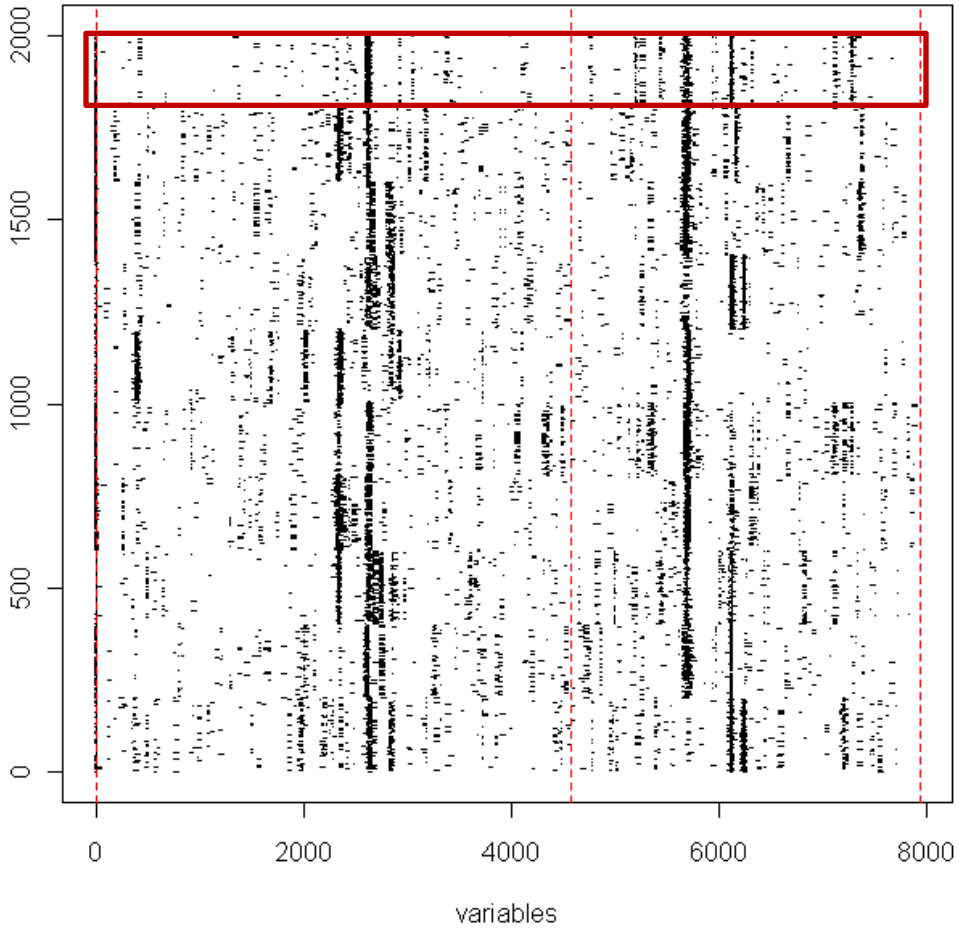

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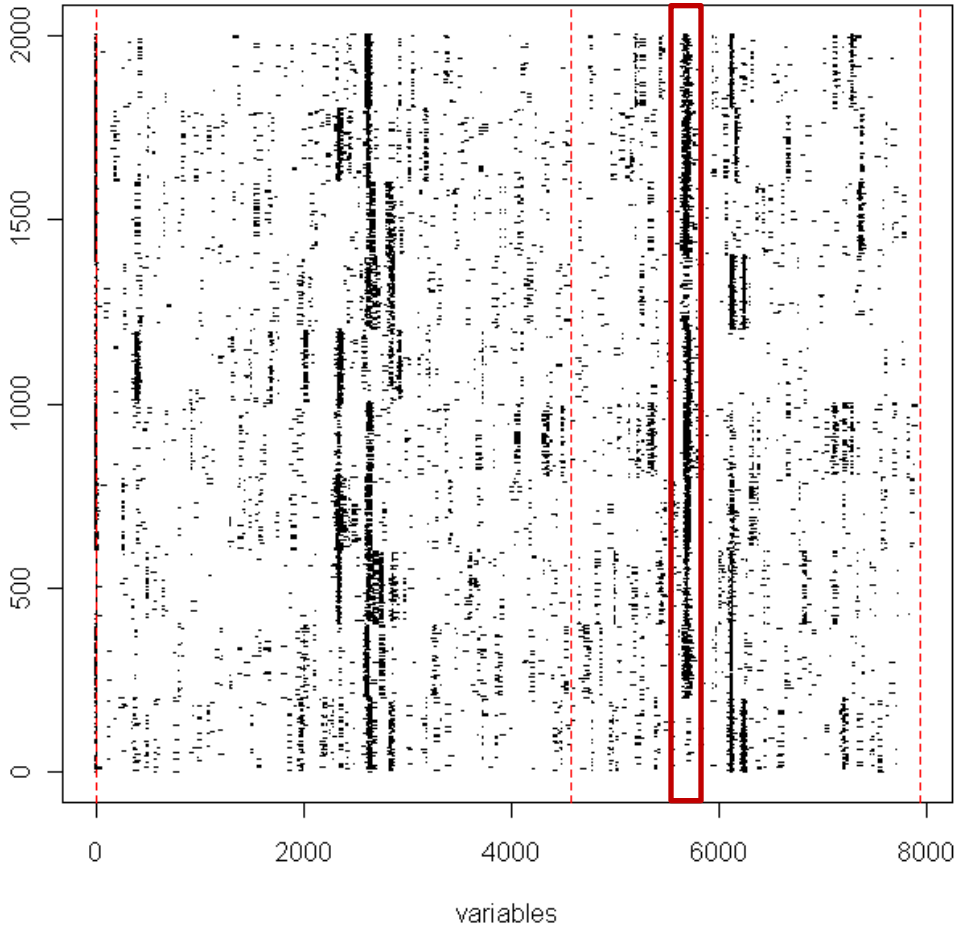

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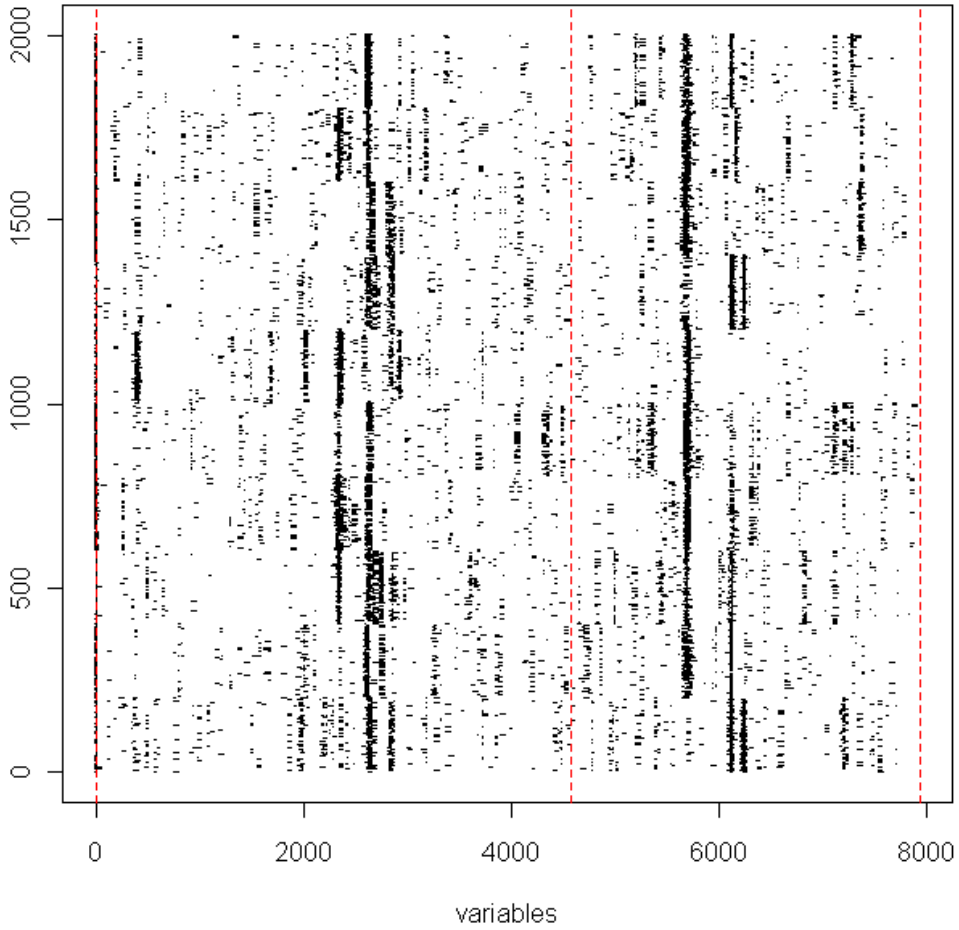

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Finally, are retained:

4 physicochemical variables
4 RAMAN intervals
2 Mid-IR intervals

$R^2=0.9936$ $R^2_{CV}=0.8273$

Results

Comparison with other methods

Necessity of feature selection ➡ comparison with PLS on all variables

Relevance of feature selection method ➡ comparison with PLS + VIP

Method	# var	# comp	R^2	R^2_{CV}
PLS	7926	7	0.7836	0.6605
PLS + VIP	4	3	0.7210	0.6650
AGvPLSm	311	12	0.9936	0.8273

Comparison of different method results (number of selected variables, number of retained components, R^2 and cross-validation R^2).

PLS — noisy model + quite bad performances

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PLS — noisy model + quite bad performances

PLS + VIP — only 4 variables (physicochemical ones)

AGvPLSm — very good model in description + cross-validation by using a reasonable number of variables split among the three tables

Conclusion

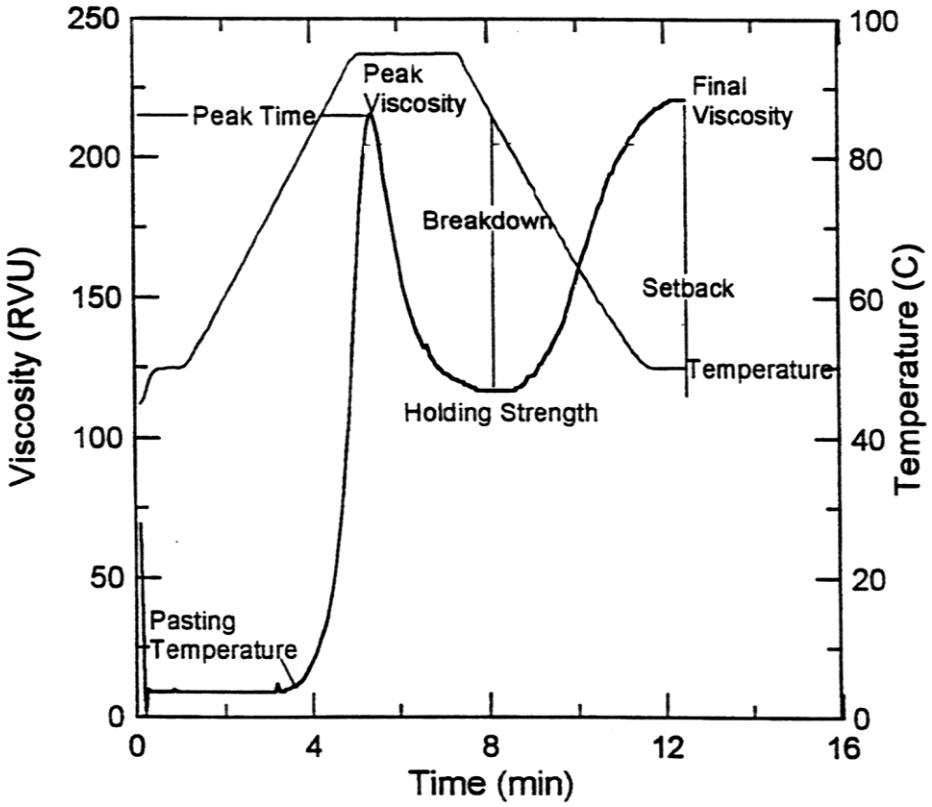
Interpretation of selected variables

1. **Physicochemical parameters**

Conclusion

Interpretation of selected variables

1. **Physicochemical parameters** → RVA



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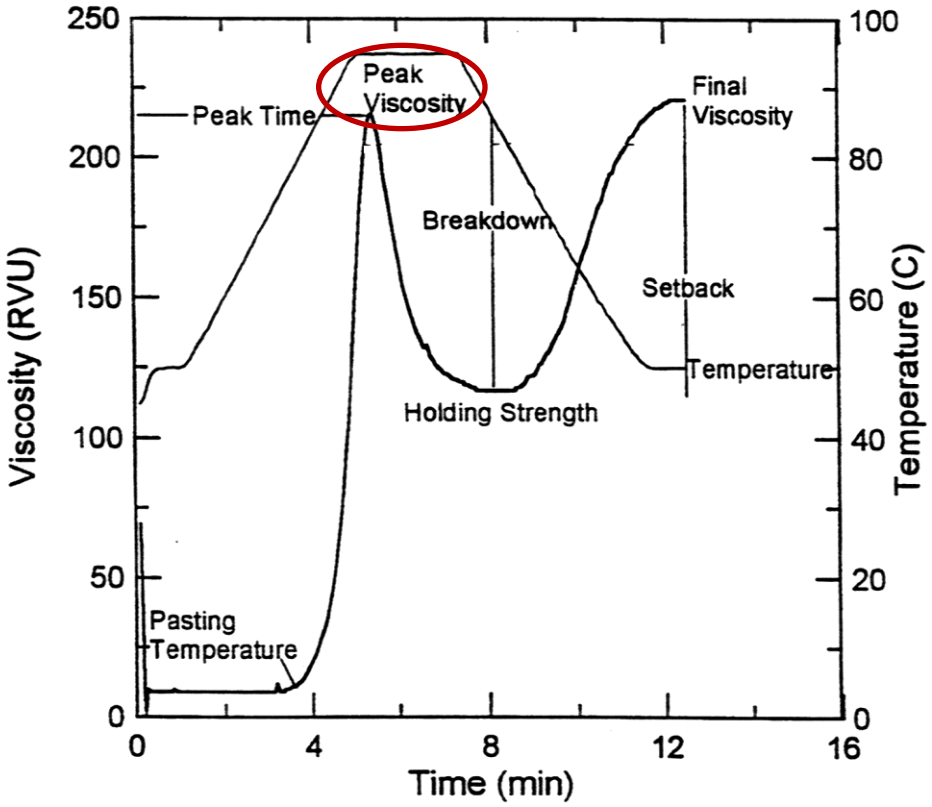

Granule size

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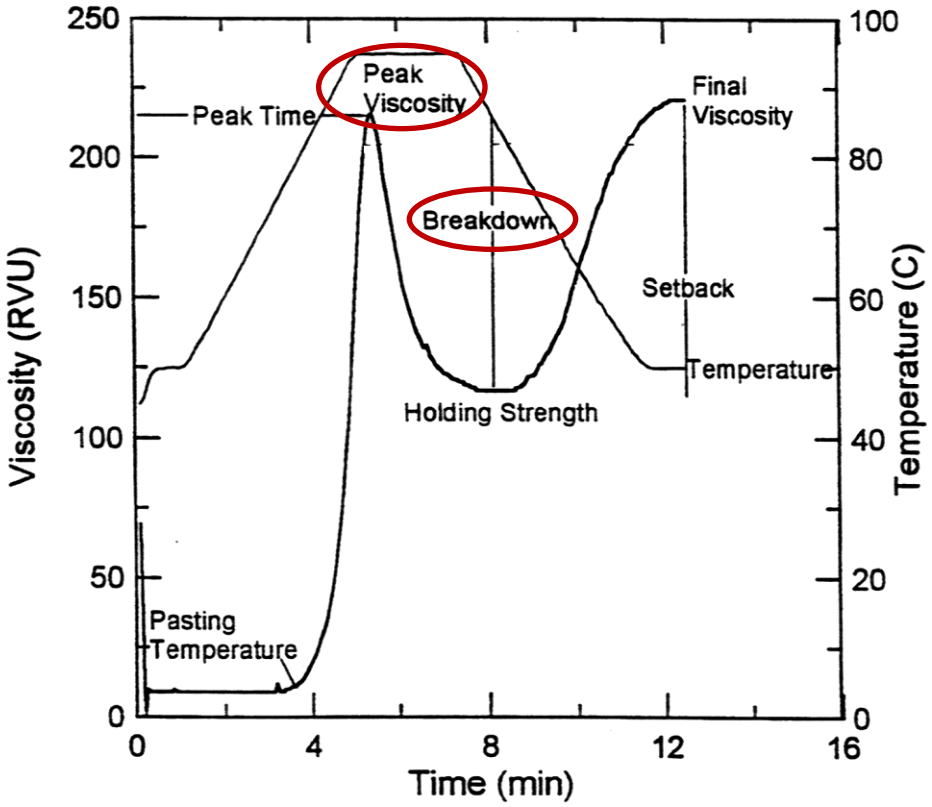

Granule size

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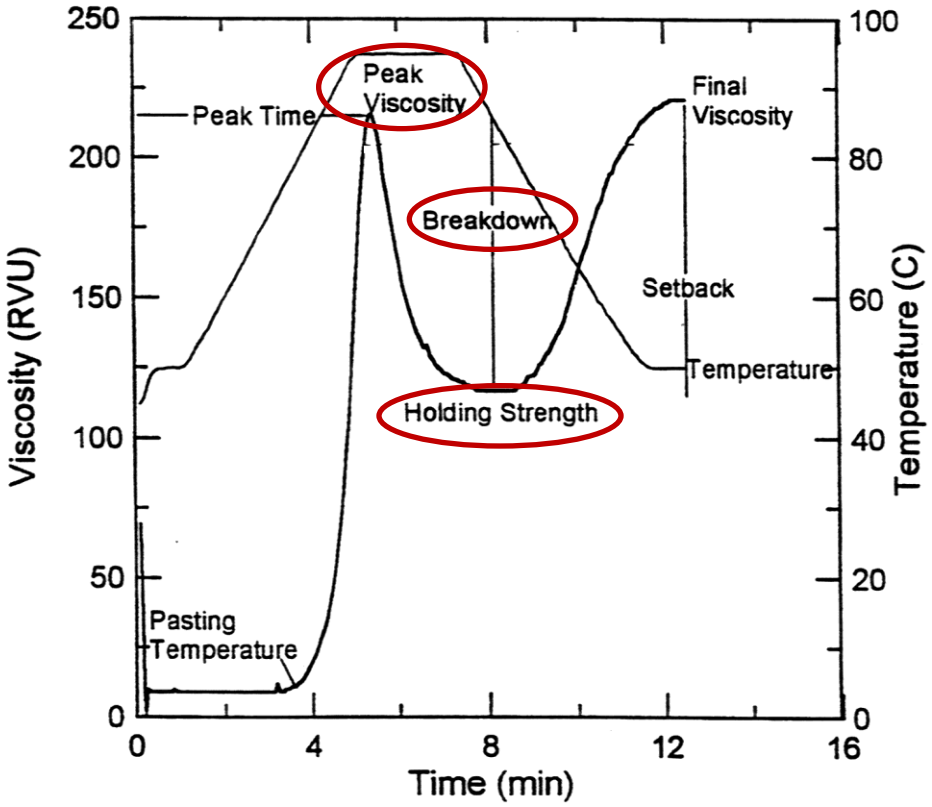

Granule size

Granule weakness

Lowest paste viscosity

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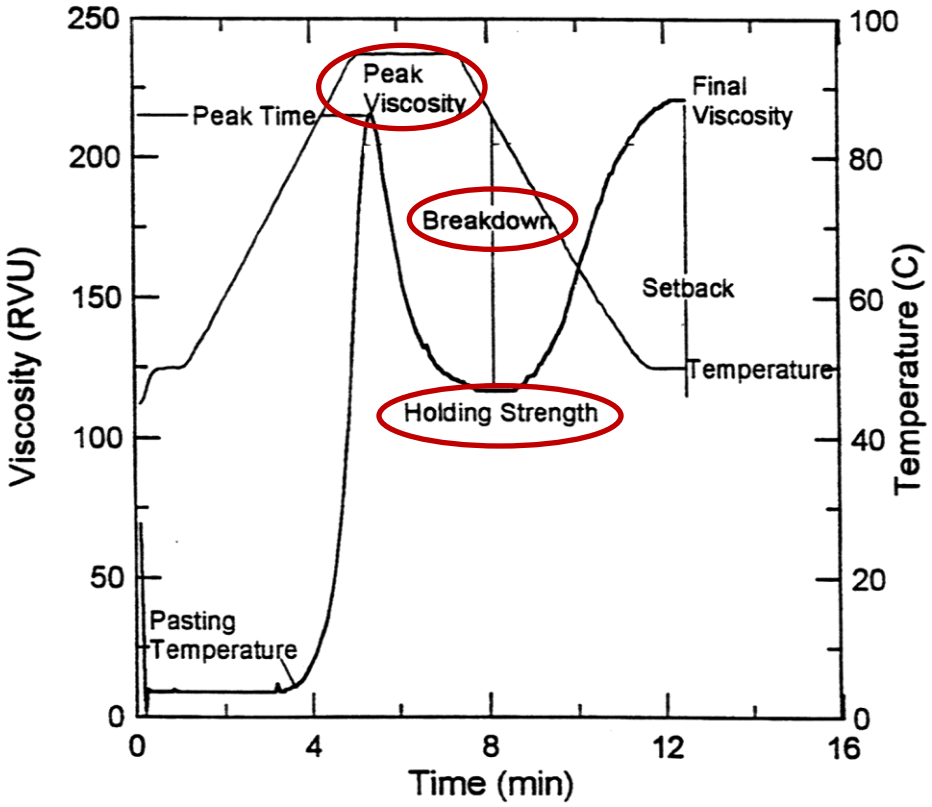

Granule size

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Lowest paste viscosity

↓

Pasting parameters

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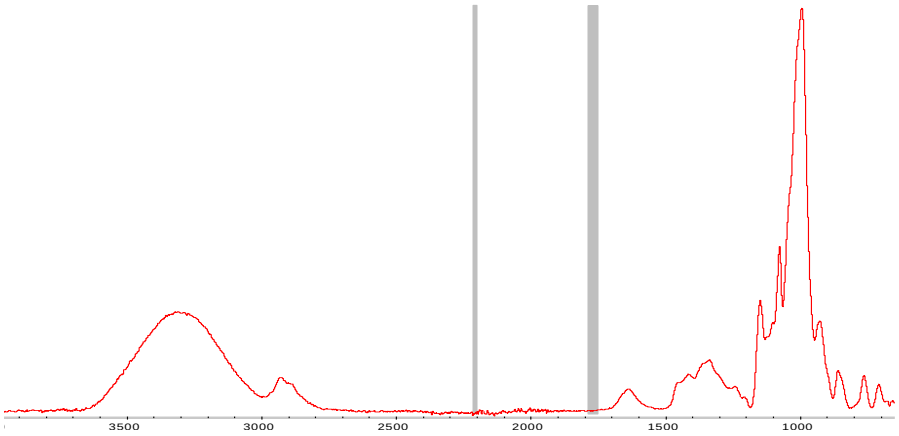
Water absorption

Conclusion

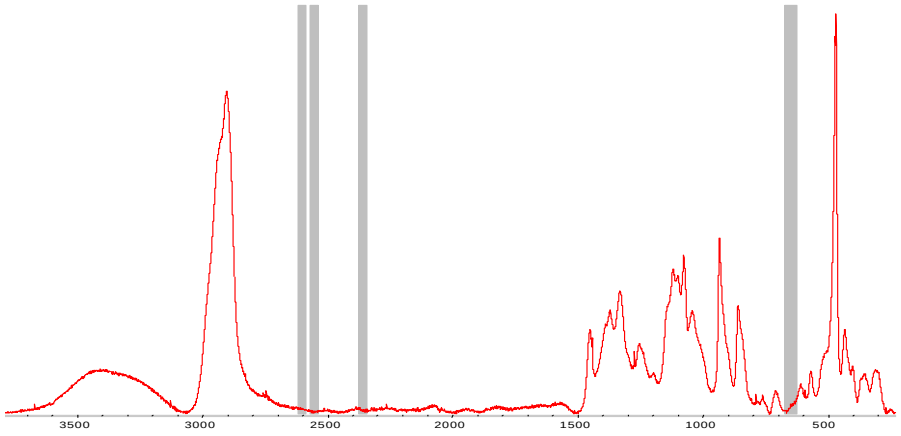
Interpretation of selected variables

1. **Spectral data** Selected variables ⇨ Intervals of wavenumbers

Mid-infrared spectra



Raman spectra

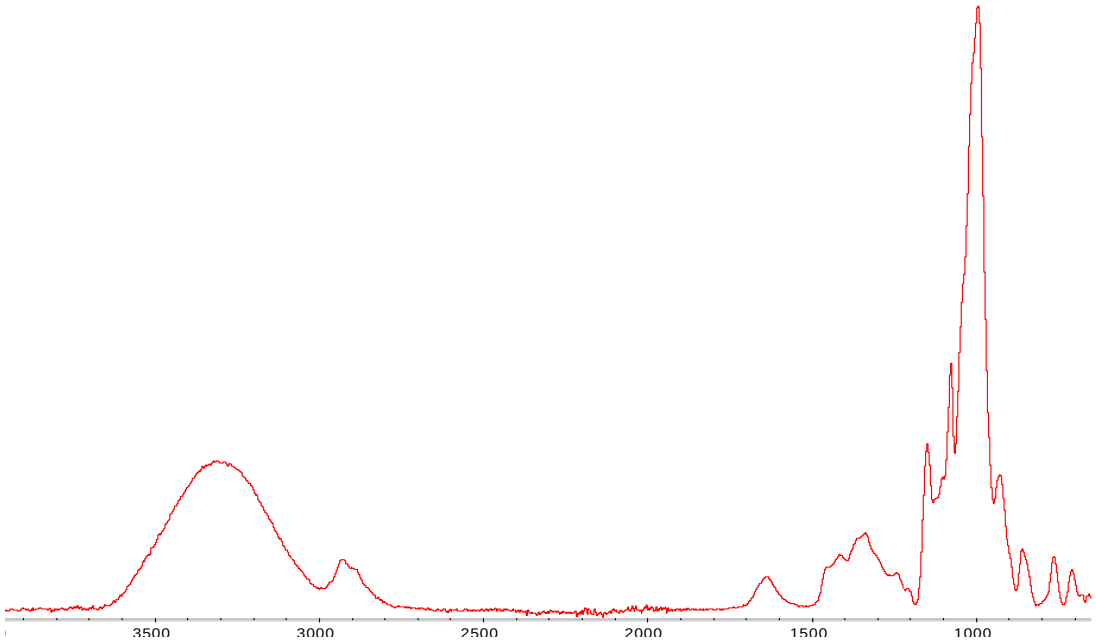


Selected range { No matching with specific vibrational bands
Improve the model

Perspectives

Perspectives

1. Constraint to the most informative areas of spectra



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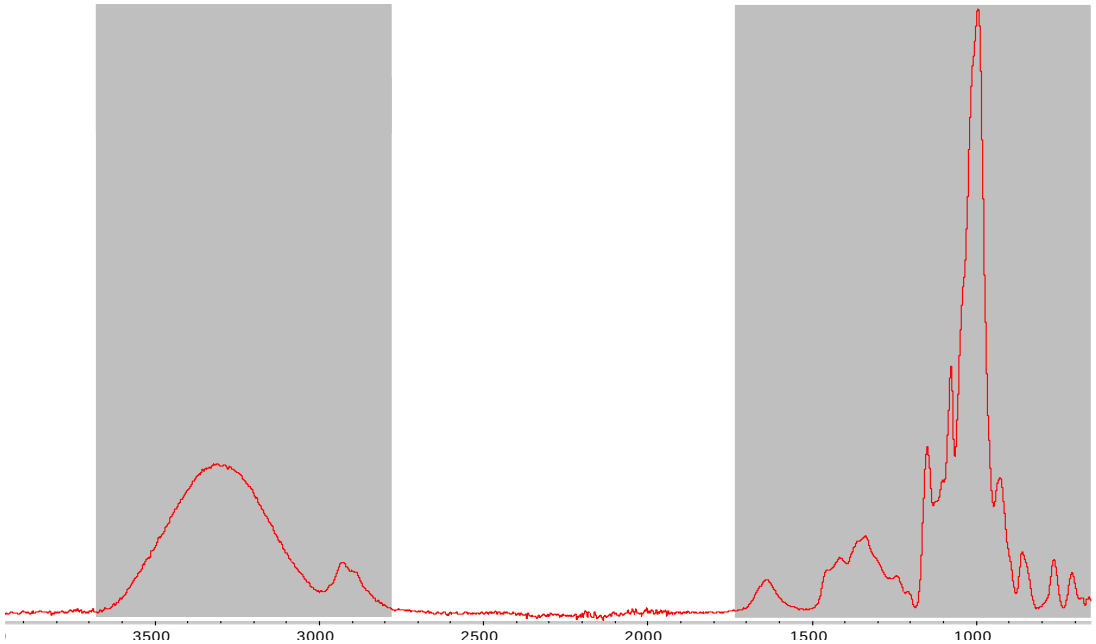
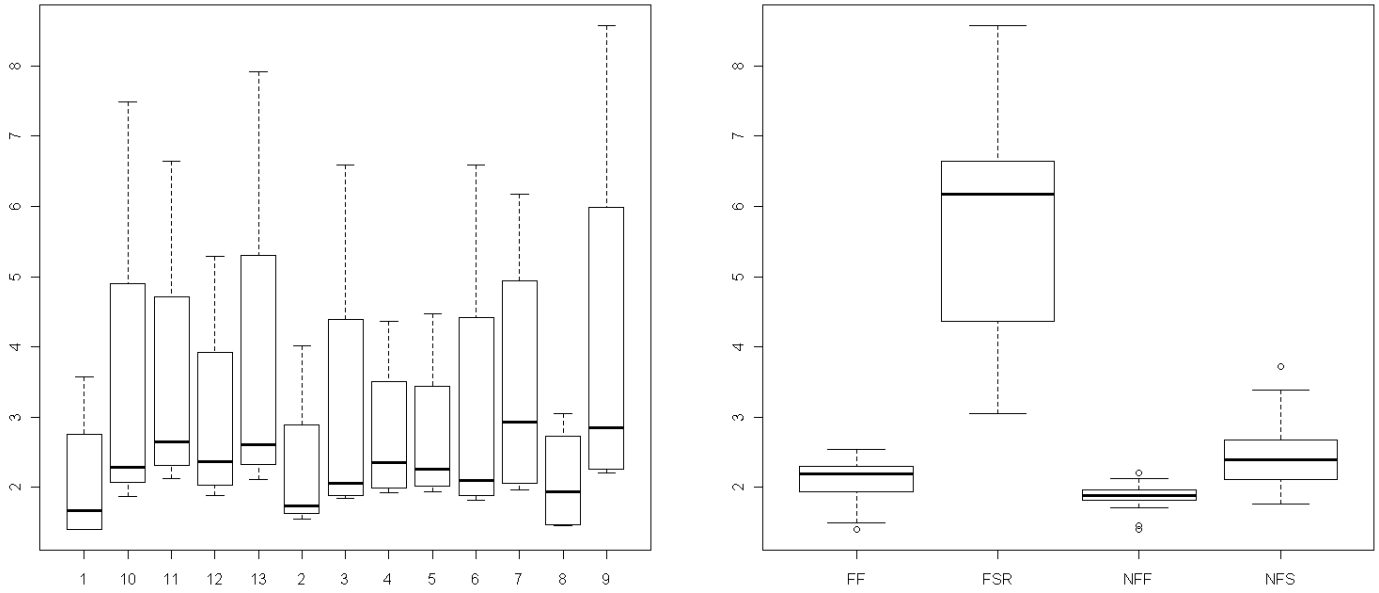


Perspectives

1. Constraint to the most informative areas of spectra

2. Collect more data → get closer to our goal and select a variety



Distribution of the breadmaking ability by variety and treatment

Aknowledgements

Thank you for your attention

Aknowledgements to

Pedro Maldonado, from Qualisud, for physicochemical data
Dominique Dufour, from CIAT in Colombia, for providing cassava starches