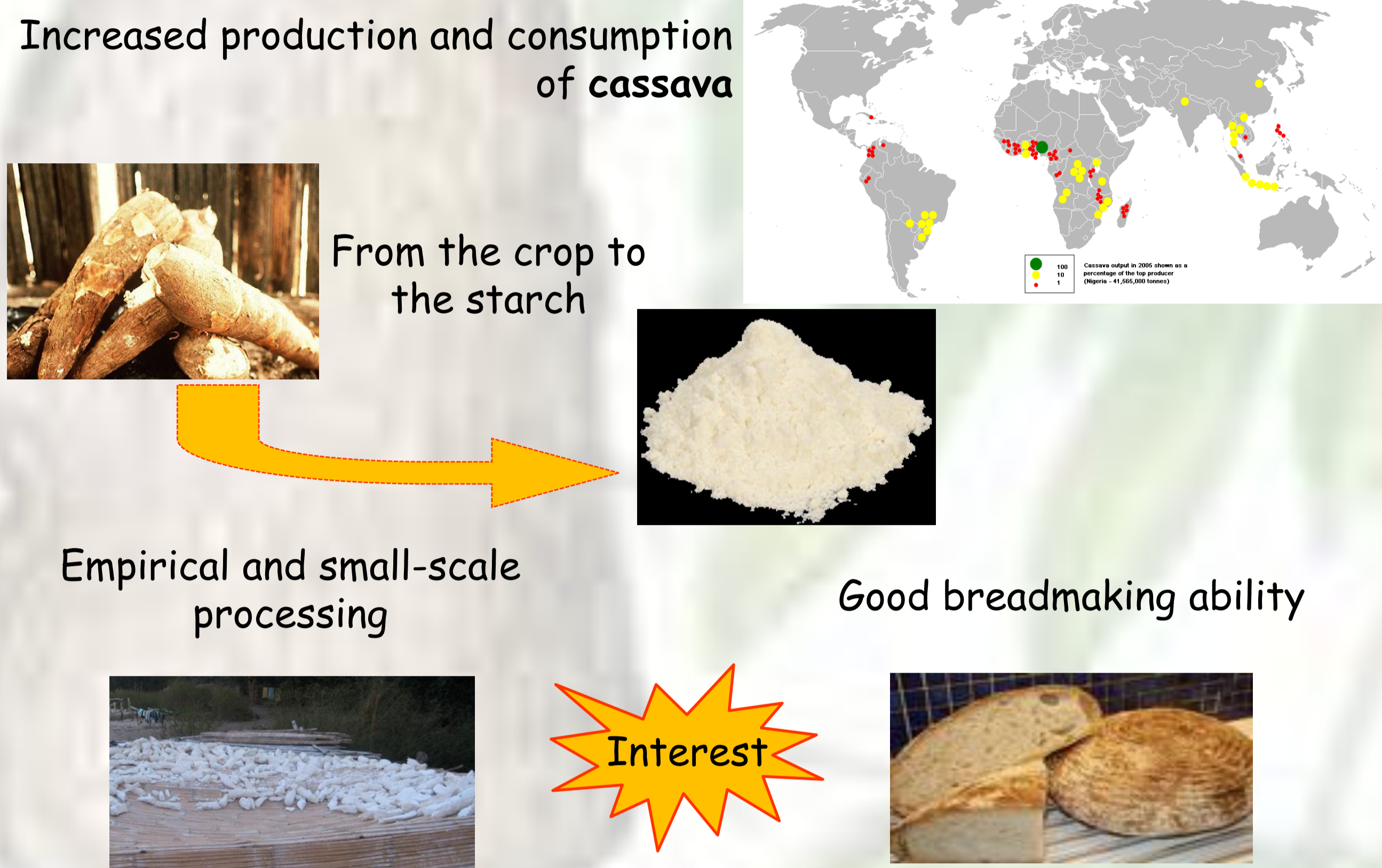


# Joint Selection of Wavenumber Regions for MidIR and Raman Spectra and Variables in PLS Regression using Genetic Algorithms

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## The Context



## The Aim



## The Data



## The Problematic

How to explain the breadmaking ability from our data using a statistical regression method while selecting variables of different types: individual and intervals?

Explanatory variables are organized in a multitables in which intervals and individual variables are selected in order to predict one variable of interest: the breadmaking capacity.

A Genetic Algorithm (GA) was developed in a context of discrimination, jointly with the PLS1 method : this method is called **selGAmPLS**.

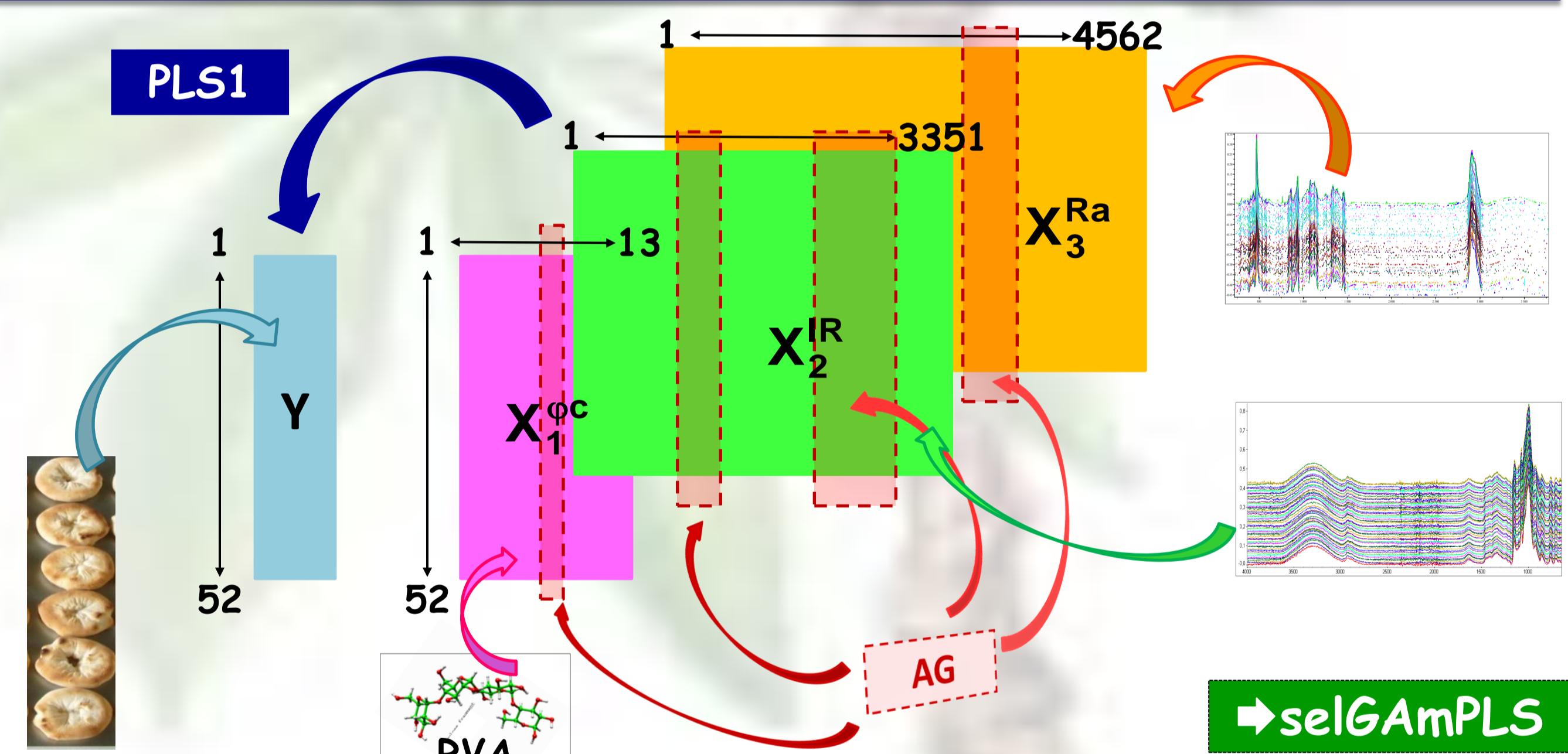
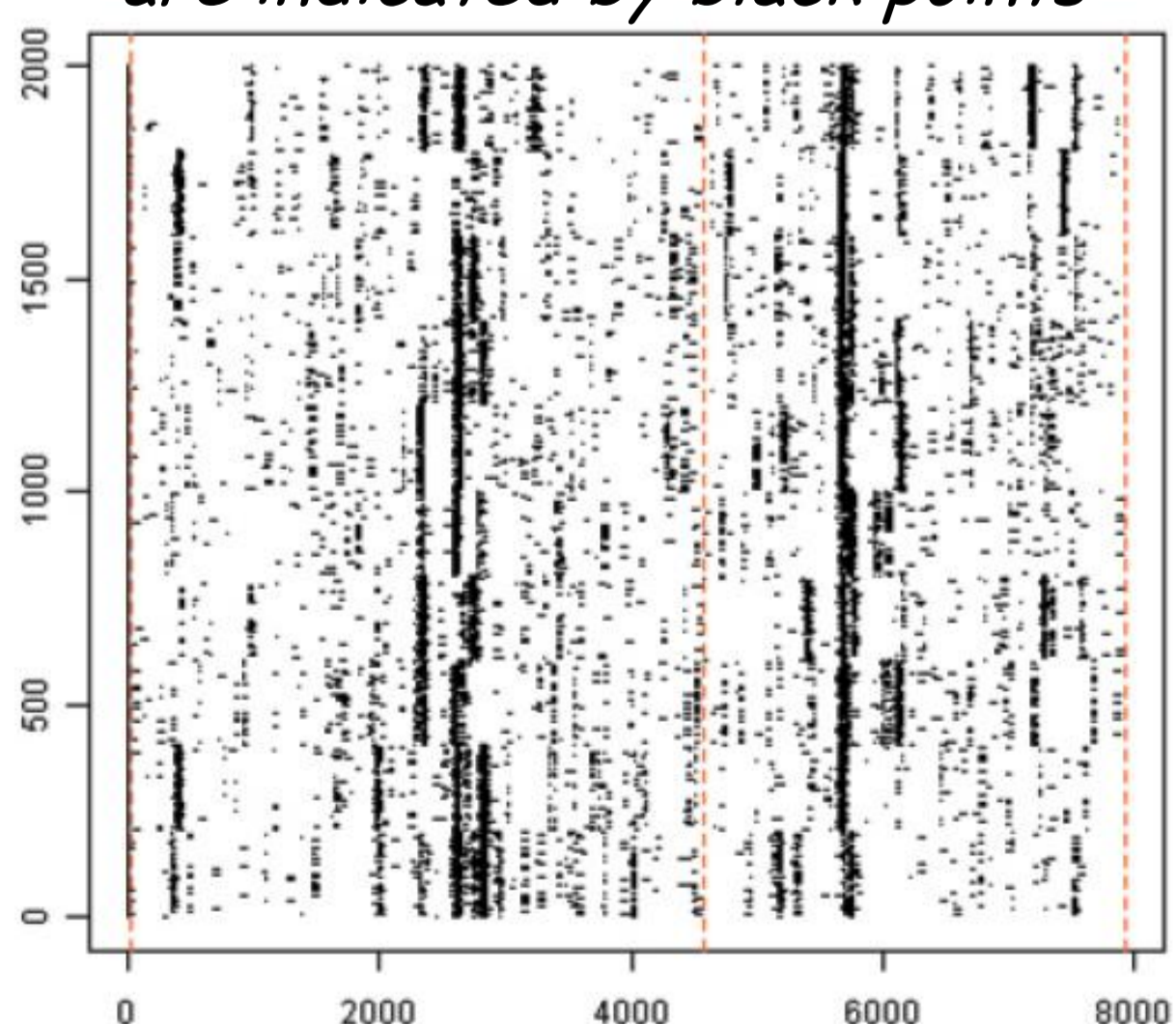


Fig 1: Selection of relevant intervals and variables in multitables with a GA for modelling Y thanks to PLS

## The Results

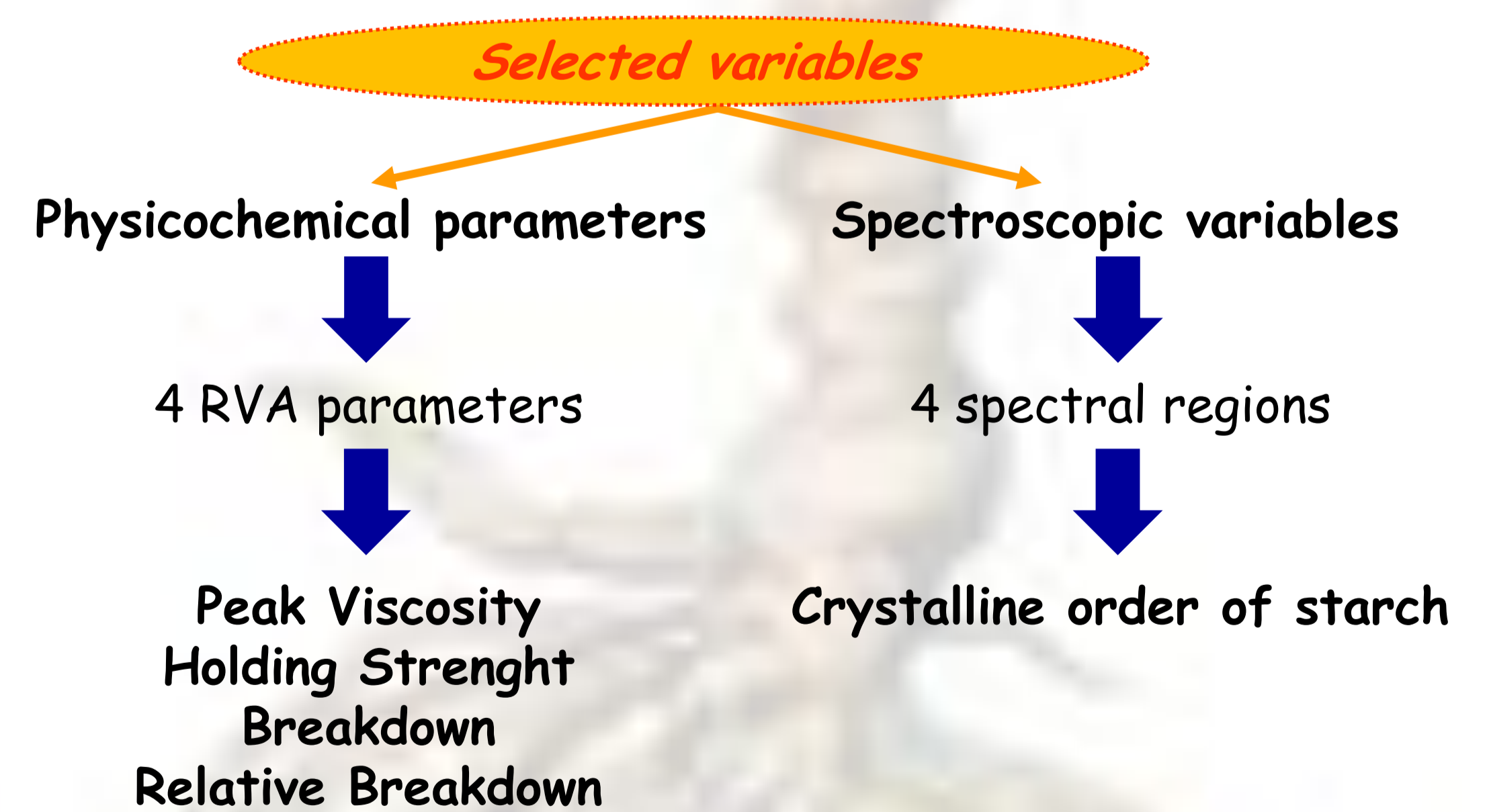
Fig 2: Final GA populations characteristics: selected variables are indicated by black points



Individual populations seem to have converged  
The 10 final populations are quite close indicating a global convergence of the GA

Table 1: Comparison with other methods results (number of selected variables, number of retained PLS components,  $R^2$  and cross-validation  $R^2$ ).

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



## Conclusion

- Genetic Algorithms provide a very adaptable and efficient solution when dealing with both several kinds of variables selections (individual vs intervals) and multiway tables.
- The results obtained are very interesting for a predictive use. In terms of interpretation the method allowed to highlight the importance of some physico-chemical variables and to select a small number of short intervals in spectroscopic data.
- The data selected are related to the water absorptivity and the crystalline state of starch and play a key role in breadmaking ability