**2. Material and methods**

2.1. Obtaining plant material

2.2. Sample preparation and FTIR measurements

2.3. Data analysis

**3. Results and discussion**

3.1. Spectroscopic analysis

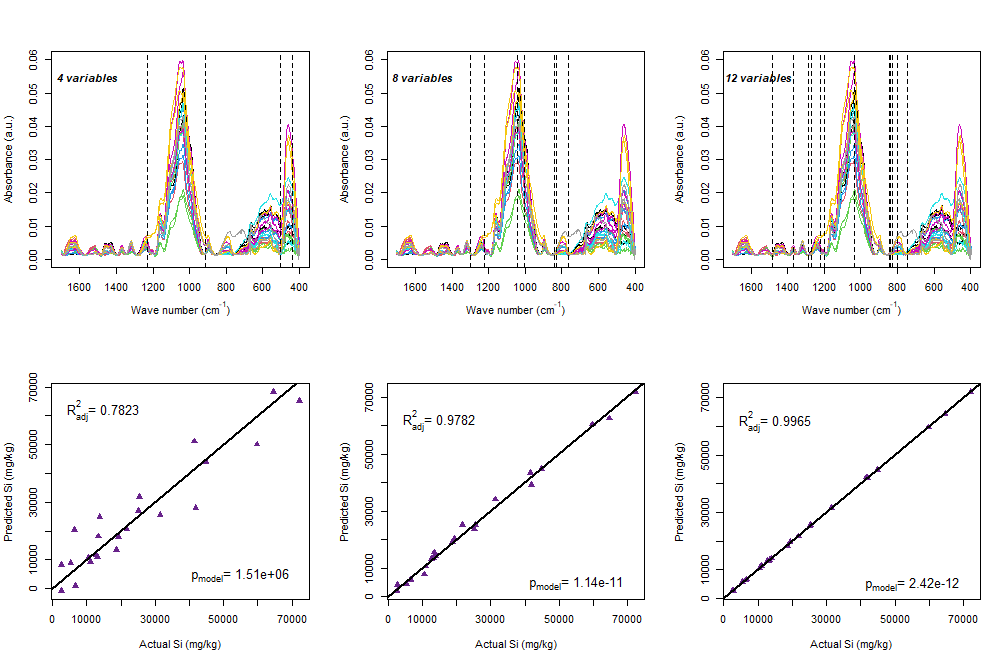
The different infrared spectra are presented in Fig. 1, where the absorption peaks of the different functional groups are observed for the species analyzed. These spectra have the following characteristic bands: a broad band at 3326, corresponding to O-H stretching vibration in phenolic and aliphatic structures, and N-H groups stretching vibration due to present proteins. Around 2917 and 2850 corresponding to CH stretching in aromatic methoxyl groups and in methyl and methylene groups of side chains. Carbonyl bands are shown around 1730, assigned to unconjugated carbonyl/carboxyl stretching.

Gráfico, Histograma

Descripción generada automáticamenteGráfico, Histograma

Descripción generada automáticamente

Figure 1: Mean infrared spectra of wheat samples (a) full mid infrared range (4000 – 400 cm-1), (b) region of interest used for calibration.

Figure 2: Mean infrared spectra of wheat leaves samples (a) after baseline correction, (b) before baseline correction.

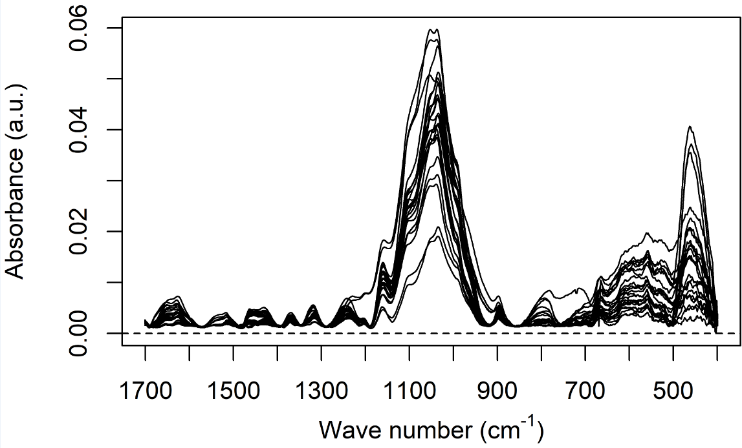
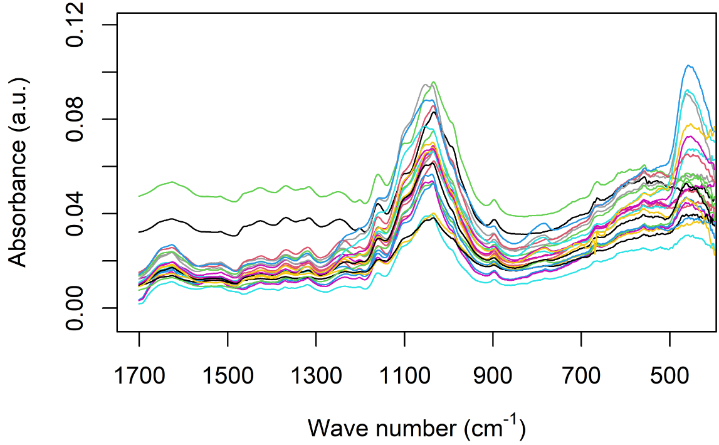


Figure 3: genetic algorithm selected variables for three different models and prediction plots for each set of variables.

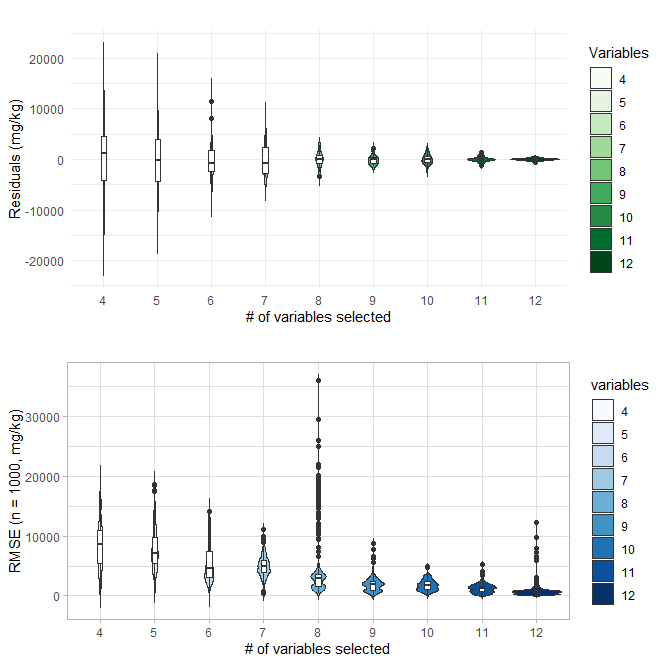


Figure 4: (a) distribution of model residuals vs complexity of model. (b) distribution of cross validated root mean squared error of prediction (folds = 10, iterations = 100) vs complexity of model.