Using infrared spectra and molecular dynamic modeling for identification of valuable molecules in olive leaves

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Currently, 4,5 million ton of olive leaves are produced annually in the world by the olive oil industry, present in southern Europe and along the Mediterranean coast. This recalcitrant biomass contains high added value bioactive chemical components. However, it represents a problem for both the farmers and the whole olive oil industry, who need to remove it from the fields and the olive oil mills. This biomass is nowadays underexploited, being burnt in the fields, given to the cattle or, in some cases, burned to produce energy.

The chemical composition of olive leaves vary depending on the species, local horticultural system or seasonal climate variations, among others. It results in high variation of the biomass suitability for the profitable biorefinery conversion. Circular bioeconomy and bio-based product development and production are becoming essential in the current transition from a fossil-based towards a new sustainable green economy. In this perspective, the possibility to valorise certain underexploited bio-based side streams and residues has huge advantages.

The goal of this research is to develop a reliable, low-cost and rapid methodology for the chemical composition determination directly in the field or sorting line. Different near infrared-based sensors and customized chemometric models were tested for this task revealing high suitability for routine application within frame of OLEAF4VALUE project. In addition an attempt for the direct interpretation of the infrared spectra was tested by means of adopting multiscale chemical-physical modelling of valuable compounds present in agricultural residuals.

**Keywords:** biomass, biorefinery, olive leaf, suitability, chemical-physical modelling

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