

P-013: HISTOCHEM: a database of reference spectra for plant cell wall polymers

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The plant cell wall is a highly organized composite made of various polysaccharides (cellulose, hemicelluloses, pectins), proteins and aromatic compounds (lignins, hydroxycinnamic acids). Determining chemical composition is a first step in cell wall characterization as it underpins its physico-chemical properties. The analyses often rely on biochemical methods, which are invasive and time consuming. Spectroscopies and microspectroscopies are alternative methods that give rapid or localized biochemical information on samples. However, spectral interpretation is complex as spectra contain features from functional groups belonging to different compounds. The analysis of spectra requires adapted data treatments methods together with spectra of almost pure and well characterized compounds and spectral bands assignments.

We present here a database named "HISTOCHEM", dedicated to FTIR spectroscopy and plant cell walls. The objective was to propose a tool making the interpretation of cell wall FTIR spectra easier for users.

The database gathers spectra of almost pure polymers and oligomers derived from cell walls and cell wall samples from different plant organs. Infrared spectra are saved under 3 different formats: spectra from 4000 to 700 cm^{-1} , spectra in the region from 2000 to 700 cm^{-1} , and second derivative spectra from 2000 to 700 cm^{-1} . Pure polymers and oligomers were characterized by wet chemistry and were used as reference samples for assignment of absorption bands to functional groups characteristic of the different compounds present in cell walls.

The database is organized around two main blocks of metadata (Figure 1). The first block contains information about samples such as the botanical origin, the tissue, the physical state and the composition. The second block concerned spectra and can be subdivided into acquisition metadata, pretreatments metadata, and spectral interpretation data: specific spectral bands and corresponding assignments with associated bibliographic references.

The database can be queried to find a spectrum from the chemical name or other kind of information stored in the database or for comparing an external spectrum with those present in the database. External spectrum can be submitted in excel format and database spectra can be exported in excel format for further processing.

Today, the database HISTOCHEM contains about 120 spectra and is still updated with new samples emerging from our own research programs or through collaborations. Soon, the database will be enriched with Raman spectra as Raman spectroscopy provides complementary information to that obtained with FTIR for the investigation of cell wall organization at the molecular level.

The database HISTOCHEM is hosted by the Plastic platform which is a software platform gathering image processing tools and databases developed at INRA [1]. The database is accessible to other lab free of charge after identification on the web application <https://pfl.grignon.inra.fr/shistochem/>

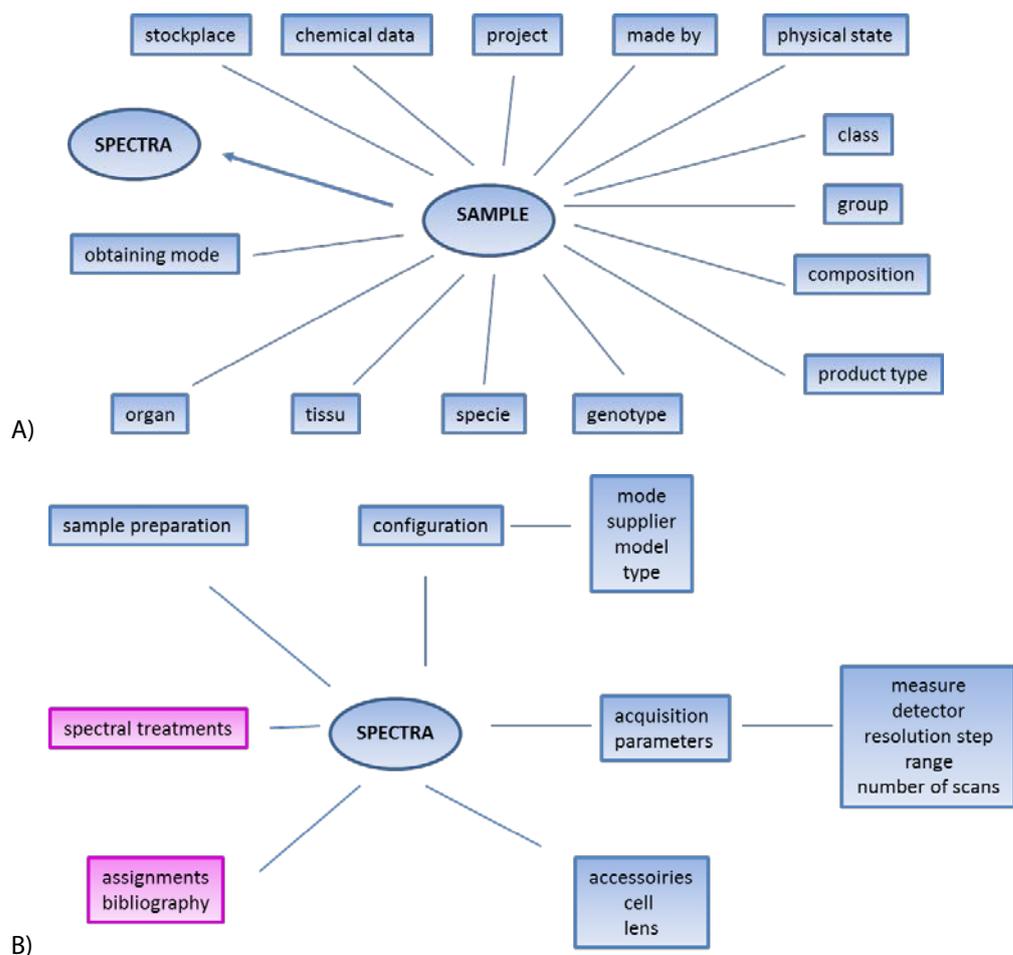


Fig. 1 metadata of the HISTOCHEM database. A) Concerning the sample used to acquire the spectra. B) Concerning the spectrum.

References

[1] <http://www.pfl-cepia.inra.fr/>