Appendix_1_list_of_organic_sample_names_of_spectra_transfer_set.tab

A set of 92 organic samples was selected to cover a large range of variation for cell wall composition to promote a wide range of spectra, in order to create spectra transfer models.

Appendix_2_transform_matrix_for_FOSS_to_BUCHI_spectra_transfer_model.tabular

The resulting spectra transfer model from FOSS to BUCHI spectra is a transform matrix allowing transforming FOSS spectra into BUCHI spectra by matrix multiplication. Other transfer models were established in a same way and transform matrices were used alike.

Appendix_3_list_of_organic_sample_names_of_spectra_transfer_validation_set.tab

A set of 11 sorghums and 24 miscanthus samples, listed in Appendix 3, was selected to validate transfer models and estimate the quality of these transfers.

Buchi-NIRFlexN500_cm-1_reflectance_spectra_transfer_set.tabular Buchi-NIRFlexN500_cm-1_reflectance_spectra_transfer_validation_set.tabular

BUCHI N500 spectrometer gave reflectance spectra in wave numbers, with a range of 4000 to 10000 cm⁻¹ and a resolution of 4 cm⁻¹. Each spectrum was an average of 96 spectral readings of the same cup or vial. Samples were poured either into 10 cm diameter cups (about 30g) or into 1.3 cm diameter vials (about 3g) and spectra were acquired in triplicate and then averaged.

FOSS-NIRSystem5000_nm_absorbance_spectra_transfer_set.tabular FOSS-NIRSystem5000_nm_absorbance_spectra_transfer_validation_set.tabular

FOSS spectrometer NIRSystem5000 gave absorbance spectra in wavelength with a range of 1100 to 2498 nm and a resolution of 2 nm. Each spectrum was an average of 32 spectral readings of the same cup. Samples were poured into 3.5 cm diameter cups (about 4g) and spectra were acquired in duplicate and automatically averaged.

ThermoScientific-ANTARIS-II_cm-1_absorbance_spectra_transfer_set.tabular ThermoScientific-ANTARIS-II_cm-1_absorbance_spectra_transfer_validation_set.tabular

ThermoScientific ANTARIS II spectrometer gave absorbance spectra in wave numbers with a range of 4000 to 10001 cm⁻¹ and a resolution of 3.86 cm⁻¹. Samples were divided into 10 subsamples (aliquots) and poured into 0.8 cm diameter vials (about 2ml) which was scanned once. For each subsample, an average (spectrum) of 64 spectra were recorded.

ChemFlow_history_spectra_transfer_model_from_FOSS_to_BUCHI.tar.gz

This folder contains all files from the ChemFlow history of the transfer function creation from FOSS to BUCHI spectra:

- Raw spectra of model set and validation set, named by "Raw...".
- Other files corresponding to output files from the transfer model workflow: sorting samples, unit conversion, absorbance/reflectance conversion.
- PDF output files corresponding to spectra plots of raw or transferred BUCHI and FOSS spectra.

Here is an image of the transfer model workflow, with all functions, created on ChemFlow (<u>https://vm-chemflow-francegrille.eu/</u>):



ChemFlow_history_spectra_transfer_model_from_BUCHI_to_FOSS.tar.gz

This folder contains all files from the ChemFlow history of the transfer function creation from BUCHI to FOSS spectra:

- Raw spectra of model set and validation set, named by "Raw...".
- Other files corresponding to output files from the transfer model workflow: sorting samples, unit conversion, absorbance/reflectance conversion.
- PDF output files corresponding to spectra plots of raw or transferred BUCHI and FOSS spectra.

Here is an image of the transfer model workflow, with all functions, created on ChemFlow (<u>https://vm-chemflow-francegrille.eu/</u>):



ChemFlow_history_spectra_transfer_model_from_BUCHI_to_ANTARIS.tar.gz ChemFlow_history_spectra_transfer_model_from_FOSS_to_ANTARIS.tar.gz ChemFlow_history_spectra_transfer_model_from_ANTARIS_to_BUCHI.tar.gz ChemFlow_history_spectra_transfer_model_from_ANTARIS_to_FOSS.tar.gz

These folders contain all files from the ChemFlow histories of the transfer function creations:

- Raw spectra of model set and validation set, named by "Raw...".
- Other files corresponding to output files from the transfer model workflow: sorting samples, unit conversion, absorbance/reflectance conversion.
- PDF output files corresponding to spectra plots of raw or transferred spectra.