P-036: NMRProcFlow: A graphical and interactive tool dedicated to 1D spectra processing for plant NMR metabolomics

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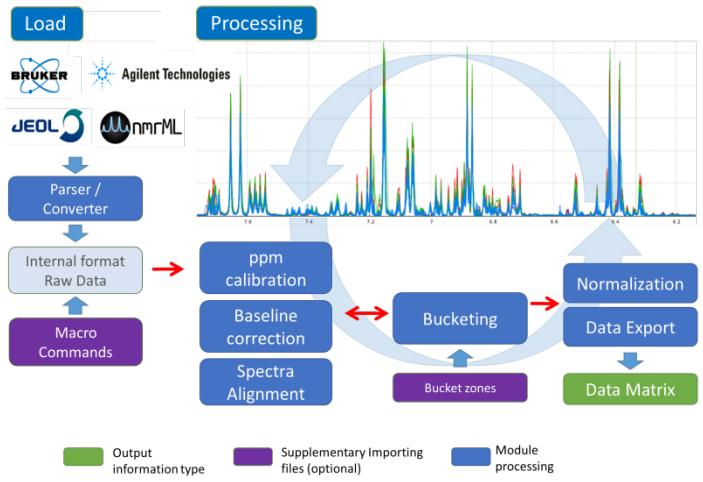
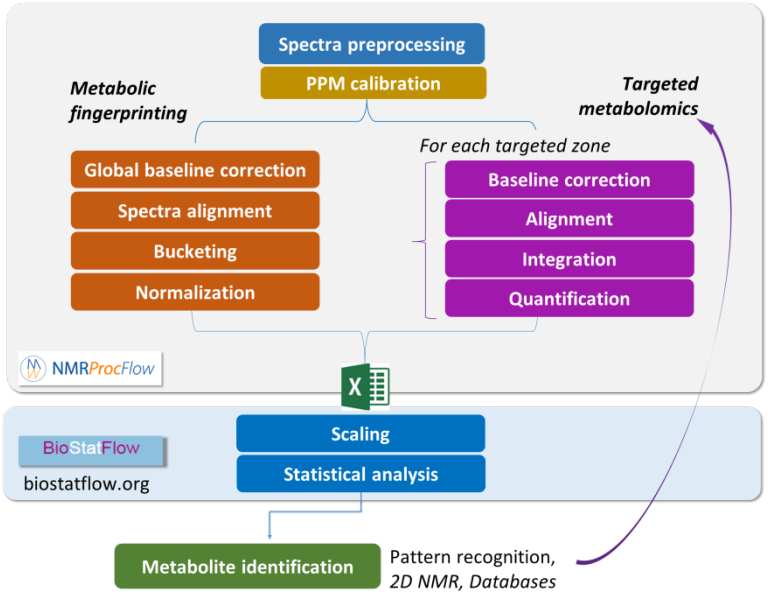
Although NMR-based metabolomics has become a common approach, multiple challenges in 1D spectra and data processing remain. Unlike separation techniques coupled with mass spectrometry for MS-based metabolomics, 1D NMR spectroscopy has only one dimension on which to rely. Apart from very well-mastered and very reproducible use-cases, the implementation of 1D NMR spectra processing workflows within a Virtual Research Environment (VRE) and operating automatically in order to be widely used by non-expert users has not yet reached full maturity. Indeed, the expert eye is often required and even crucial to disentangle the intertwined peaks and the best way is to proceed interactively with a 1D NMR spectra viewer.



NMRProcFlow covers all spectra processing steps including baseline correction, chemical shift calibration and alignment

To fulfill this need, we have been developing NMRProcFlow [1], an interactive 1D NMR spectra processing (^{1}H or ^{13}C) dedicated to metabolomics. It has been built by involving NMR spectroscopists eager to have a quick and easy tool that greatly helps spectra processing, and can be used by new-comers also.

For each of the two major metabolomics approaches, namely metabolic fingerprinting and targeted metabolomics, the workflow covers all steps from spectral data preprocessing up to data matrix export.



For Metabolic Finger-printing or Targeted Metabolomics, NMRProcFlow workflow covers all steps from spectral data to data matrix

Moreover, the possibility of visualizing the experimental factor levels within the NMR spectra set through a spectral viewer makes the tool valuable to create links between the experimental design and subsequent statistical analyses, and thus facilitates interactions between biologists and NMR spectroscopists. In addition, NMRProcFlow allows experts to build their own spectra processing workflows, in order to become "models" applicable to similar NMR spectra sets, *i.e.* stated as use-cases.

NMRProcFlow handles Bruker, JEOL, Varian and nmrML formats. It is accessible online (http://nmrprocflow.org), or alternatively, a virtual machine for local installation can be downloaded.

NMRProcFlow has been used in several plant projects including studies on tomato fruit [2] and maize grain [3].

References

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Acknowledgments

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