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NMRProcFlow: A graphical and interactive tool dedicated to batch processing of 1D spectra for NMR-based metabolomics and qNMR analysis

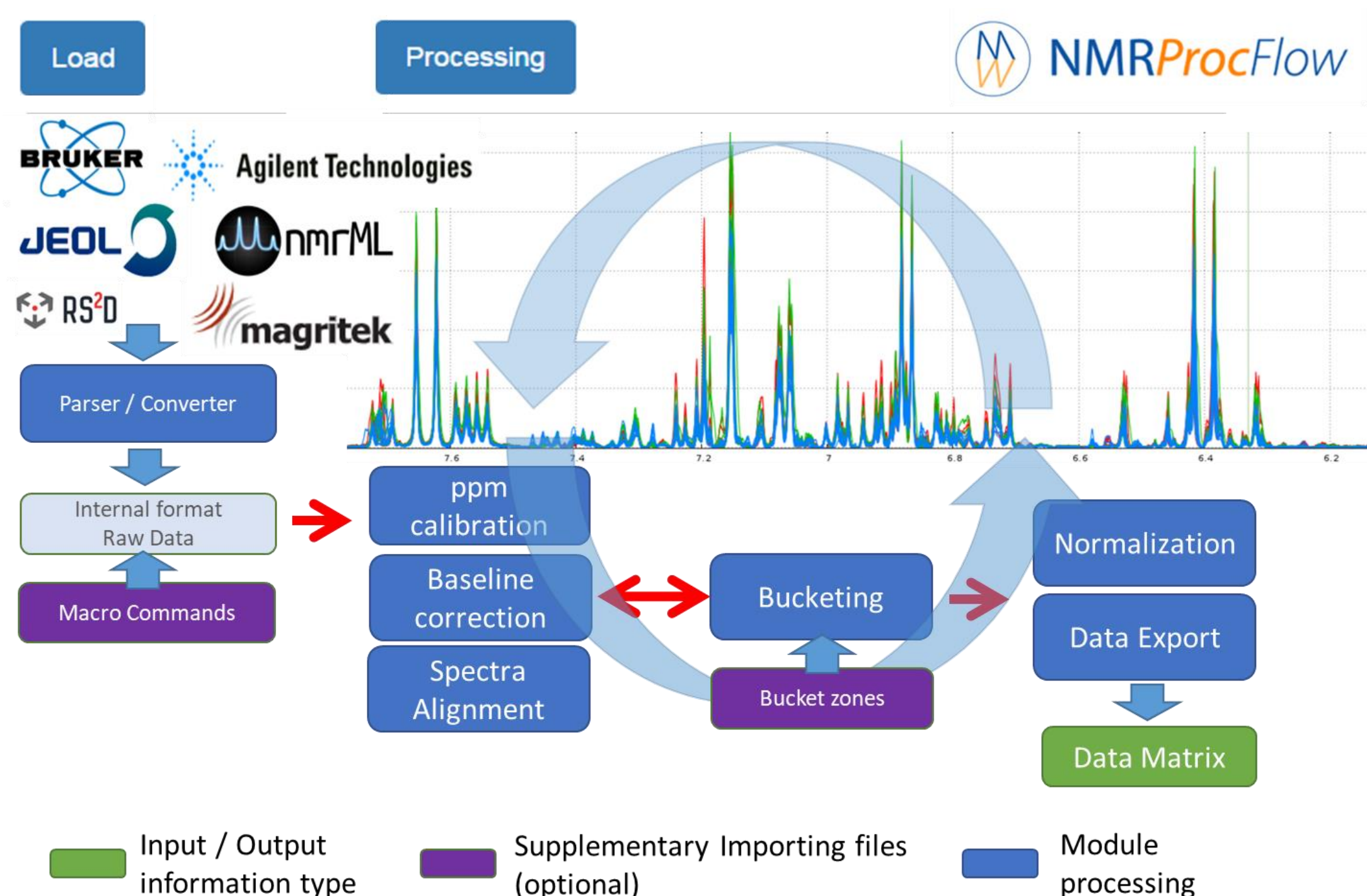
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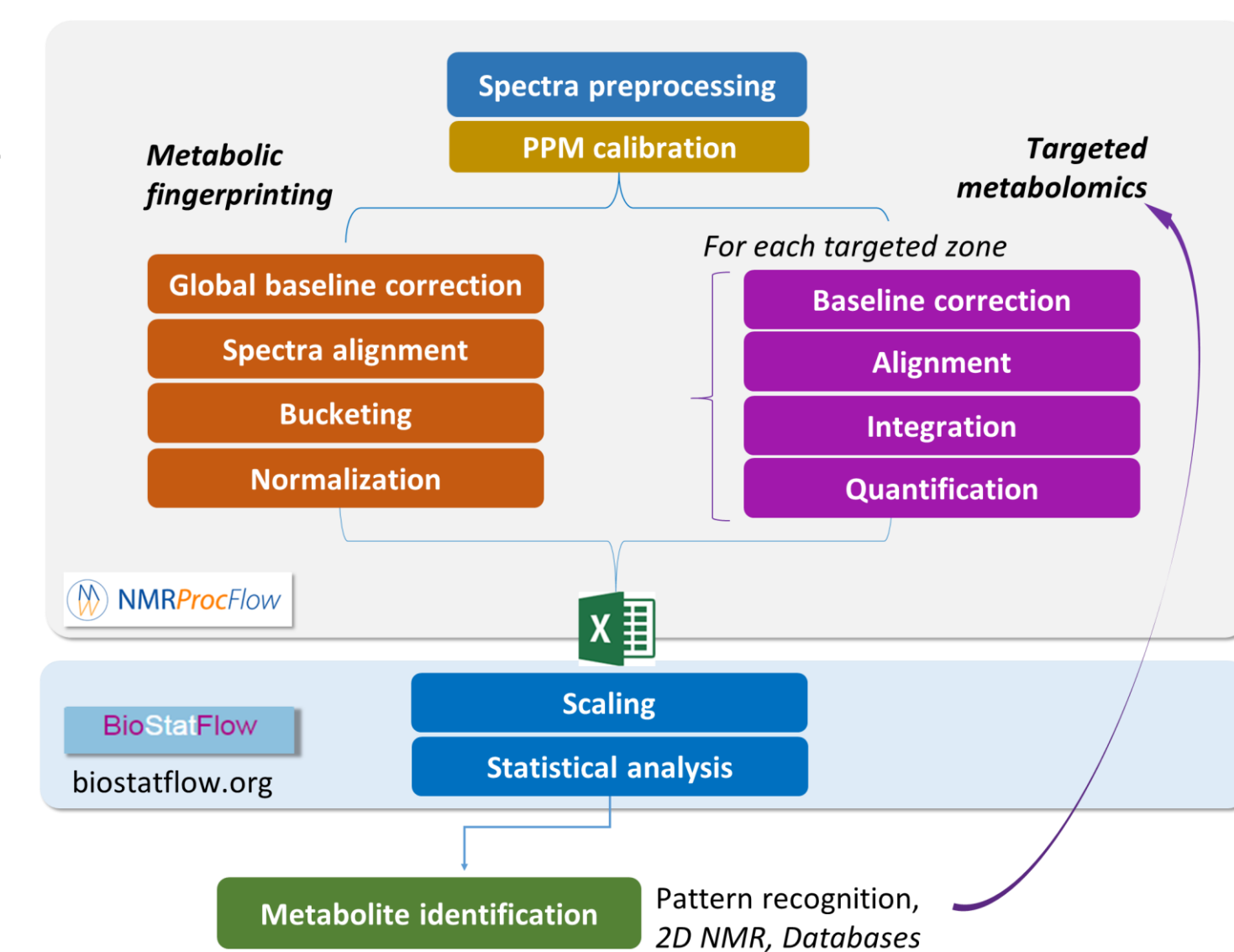
NMRProcFlow: a graphical and interactive tool for processing and visualizing 1D NMR data



Because the expert eye is often required and even crucial to disentangle intertwined or partially overlapped peaks and especially certain uncontrolled peak shifts in a set of ¹H spectra, the best way is to proceed interactively with a 1D NMR spectra viewer.

To fulfill this need, we have been developing NMRProcFlow (Jacob et al. 2017):

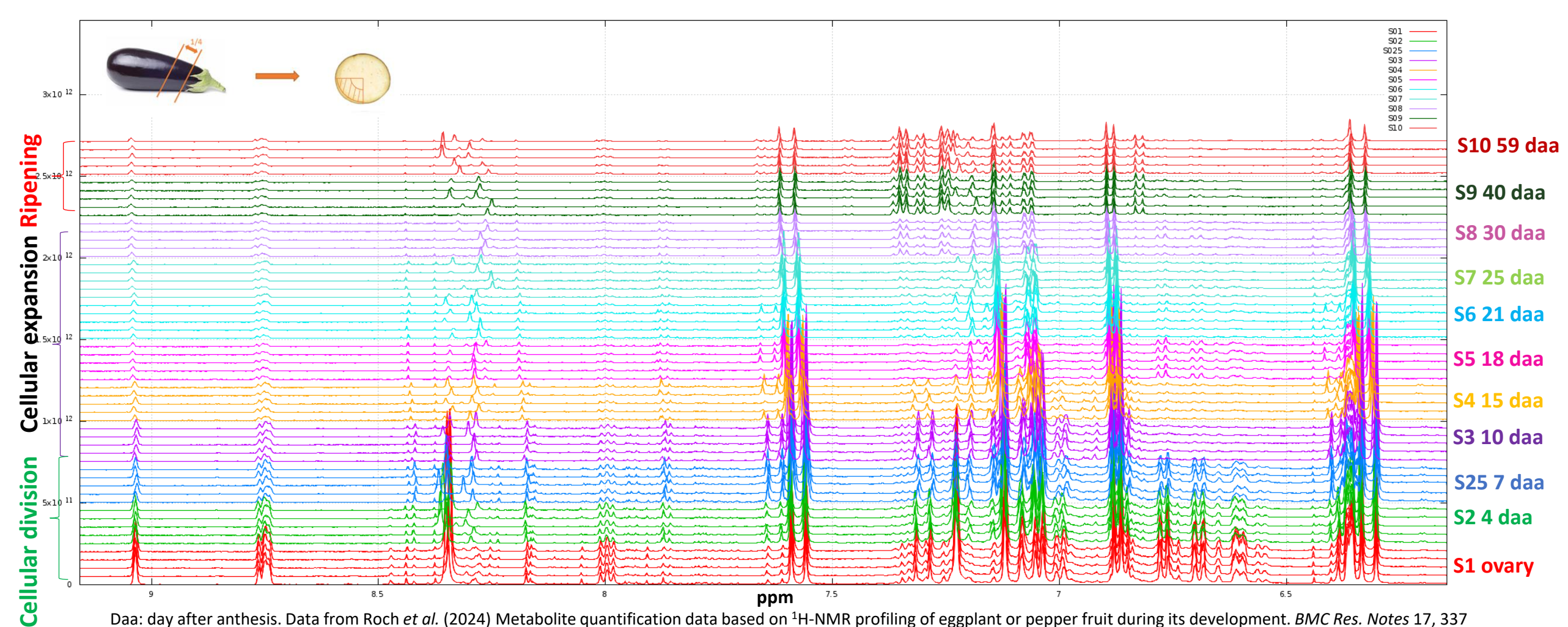
- an interactive tool for 1D NMR spectra (¹H, ¹³C & ³¹P) processing dedicated to metabolomics,
- built by involving NMR spectroscopists eager to have a quick and easy tool that greatly helps spectra processing and can be used by new-comers also,
- aiming to help NMR processing without the need for programming skills, in a graphical and interactive way.



Metabolomics

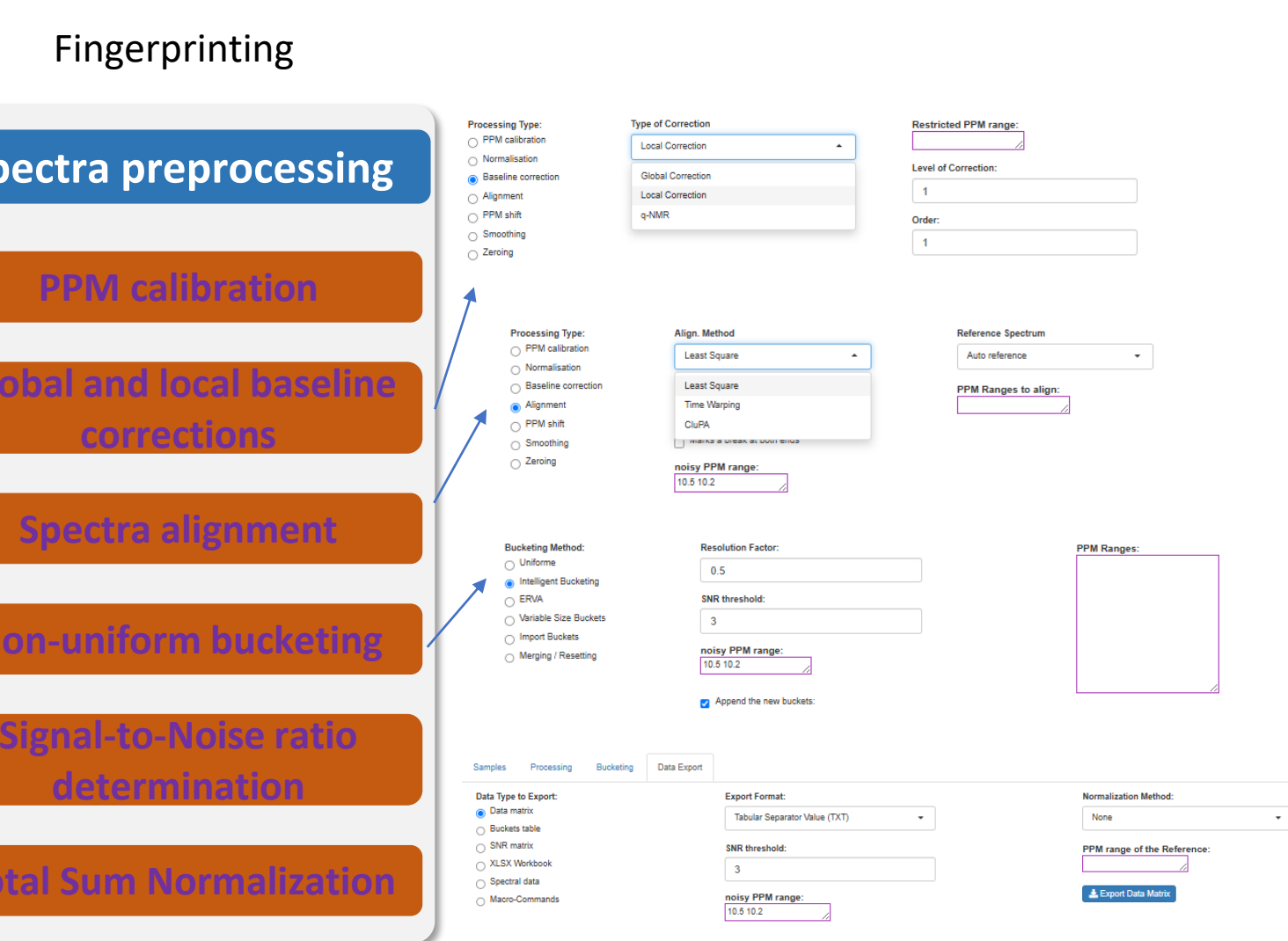
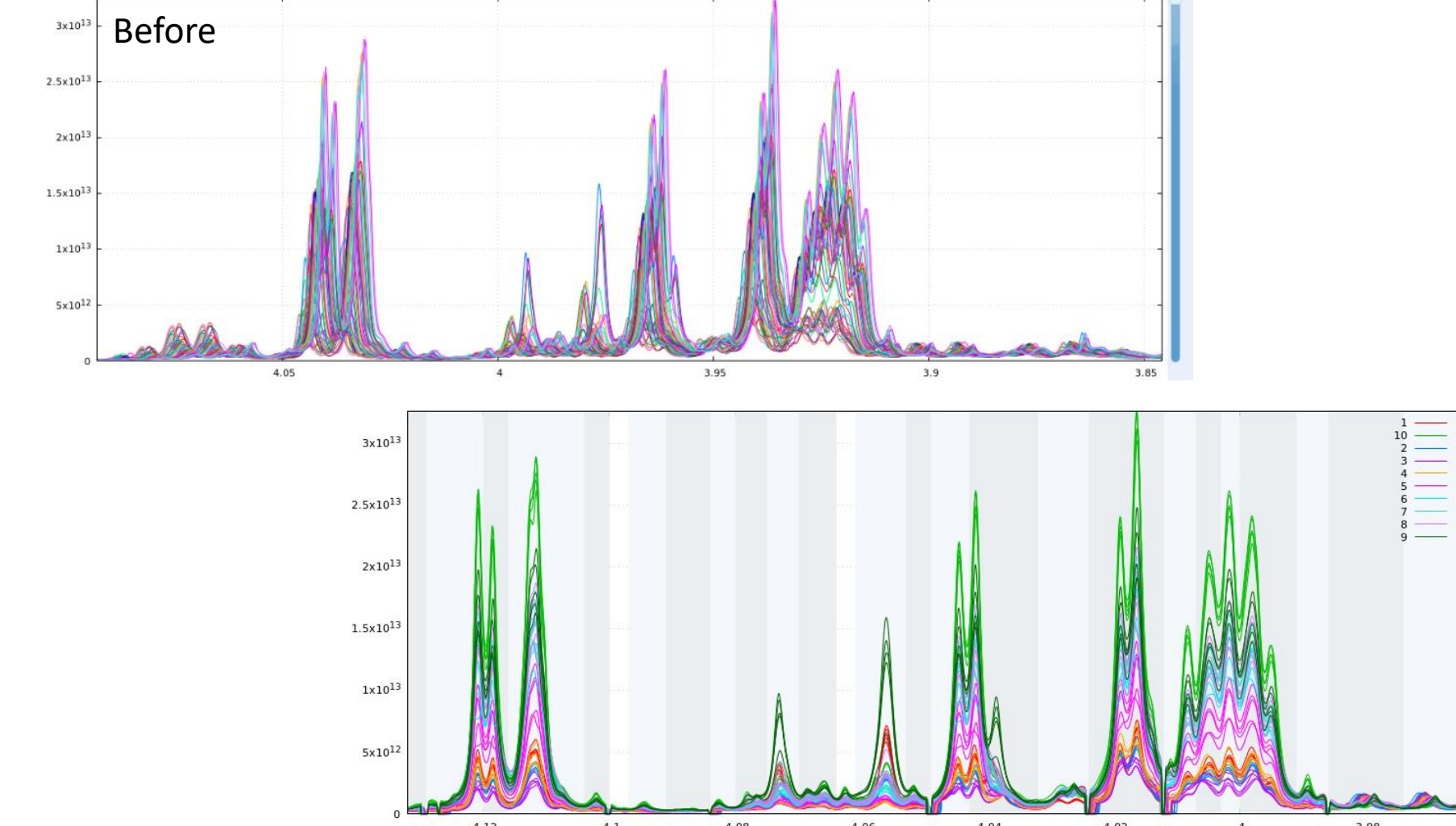
NMRProcFlow Visualisation according to experimental factors: e.g. fruit developmental stages

55 samples of Eggplant pericarp extracts
11 developmental stages



1D spectra processing tool for fingerprinting

50 samples of pepper pericarp extracts
10 developmental stages



“Use of automated softwares delivering assigned and quantified data without reference to the NMR spectra has resulted in increasing numbers of publications with incorrect assignments and consequently wrong biological interpretation of results. Some softwares, e.g. NMRProcFlow (Jacob et al. 2017) have developed preprocessing pipelines to encourage users to visualize the NMR spectra.”

Loo RL, Mosquera JO, Zasso M, Mathews J, Johnston DG, Nicholson JK, Patiny L, Holmes E, Wist J. (2024) MetaboScope: a statistical toolbox for analyzing ¹H nuclear magnetic resonance spectra from human clinical studies. *Bioinform. Adv.* 4:vbae142. doi: [10.1093/bioadv/vbae142](https://doi.org/10.1093/bioadv/vbae142)

qNMR

NMRProcFlow used for quantification of e.g.:

- ascorbic acid in acerola-based food supplements (Bourafai-Aziez et al. 2022)
- carnosic acid in *Salvia rosmarinus* (lobbi et al. 2023)
- a range of metabolites in urine (Canlet et al. 2023)
- pyroglutamic acid in wine (Watson et al. 2025)
- a range of metabolites in fruits (Roch et al. 2020, 2024)
- a range of polar and lipid compounds in feed for insect rearing (Melis et al. 2019; Anedda et al. 2023)
- major quaternary-ammonium metabolites in boxwood leaf (Hay et al. 2024)

Authenticity

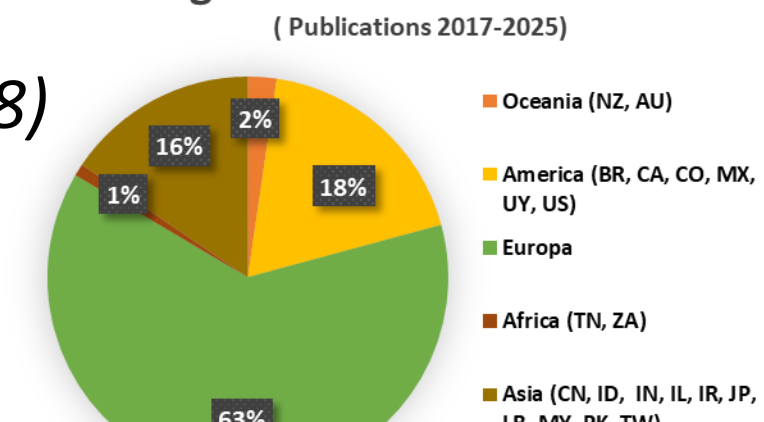
WAP-NMR project (ANR-21-CE21-0014): ¹H NMR metabolomics approach for assessing wine authenticity (Leleu et al. 2024).

- Development of a package dedicated to 1D proton NMR quantification based on peak fitting, quantification profile and external calibration
- See Poster RnmrQuant1D, D. Jacob.

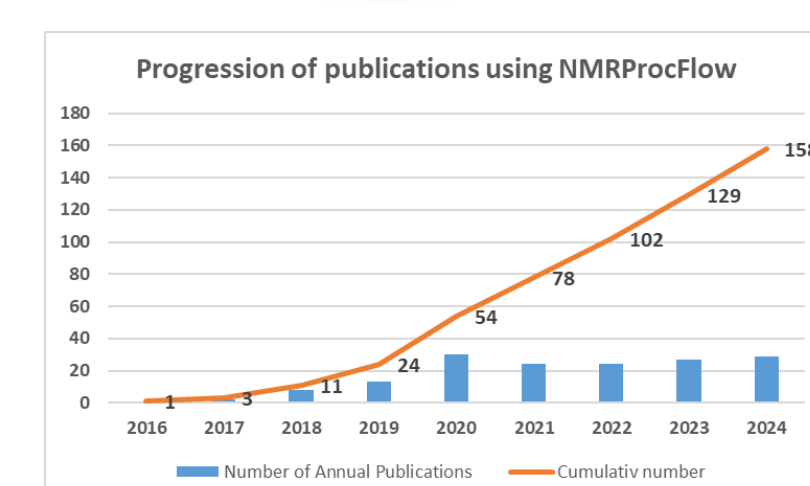
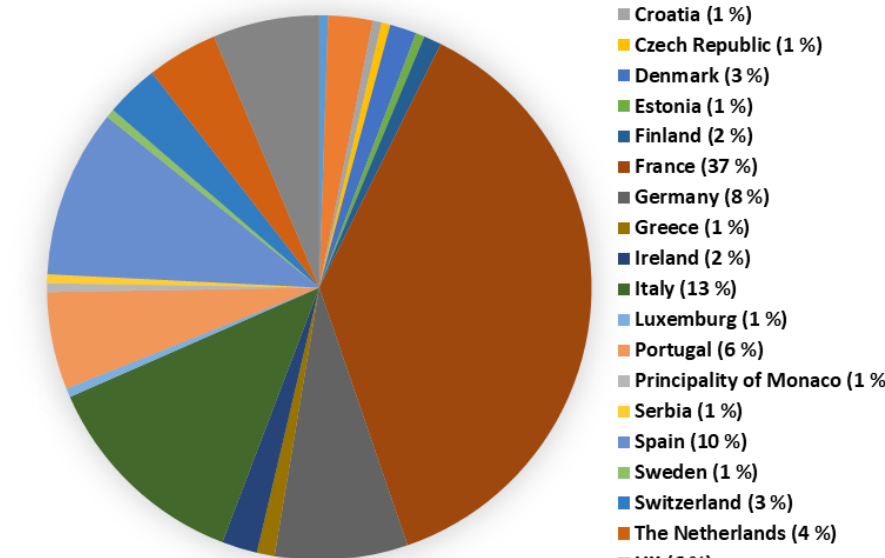
NMRProcFlow in numbers

- Virtual machine for local installation or online instance (Jacob et al. 2018)
- 4,000 sessions per year on the nmrprocflow.org online instance
- Users from the five continents
- 158 publications using NMRProcFlow for fingerprinting, qNMR, SNR
- Cited in 21 review articles (Web of Science Core Collection) 2017-2025

Origin of NMRProcFlow users (Publications 2017-2025)



Europa Users



Conclusions & Perspectives

NMRProcFlow is used by the international NMR-based metabolomics community and beyond:

- for 1D-NMR fingerprinting, relative or absolute quantification, signal-to-noise ratio determination in batch
- in different fields of science: Biology, Chemistry, Physics
- online, or locally by downloading a virtual machine (Jacob et al. 2018)
- for solid-state 1D-NMR processing in batch: on-going development.

References

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