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Introduction

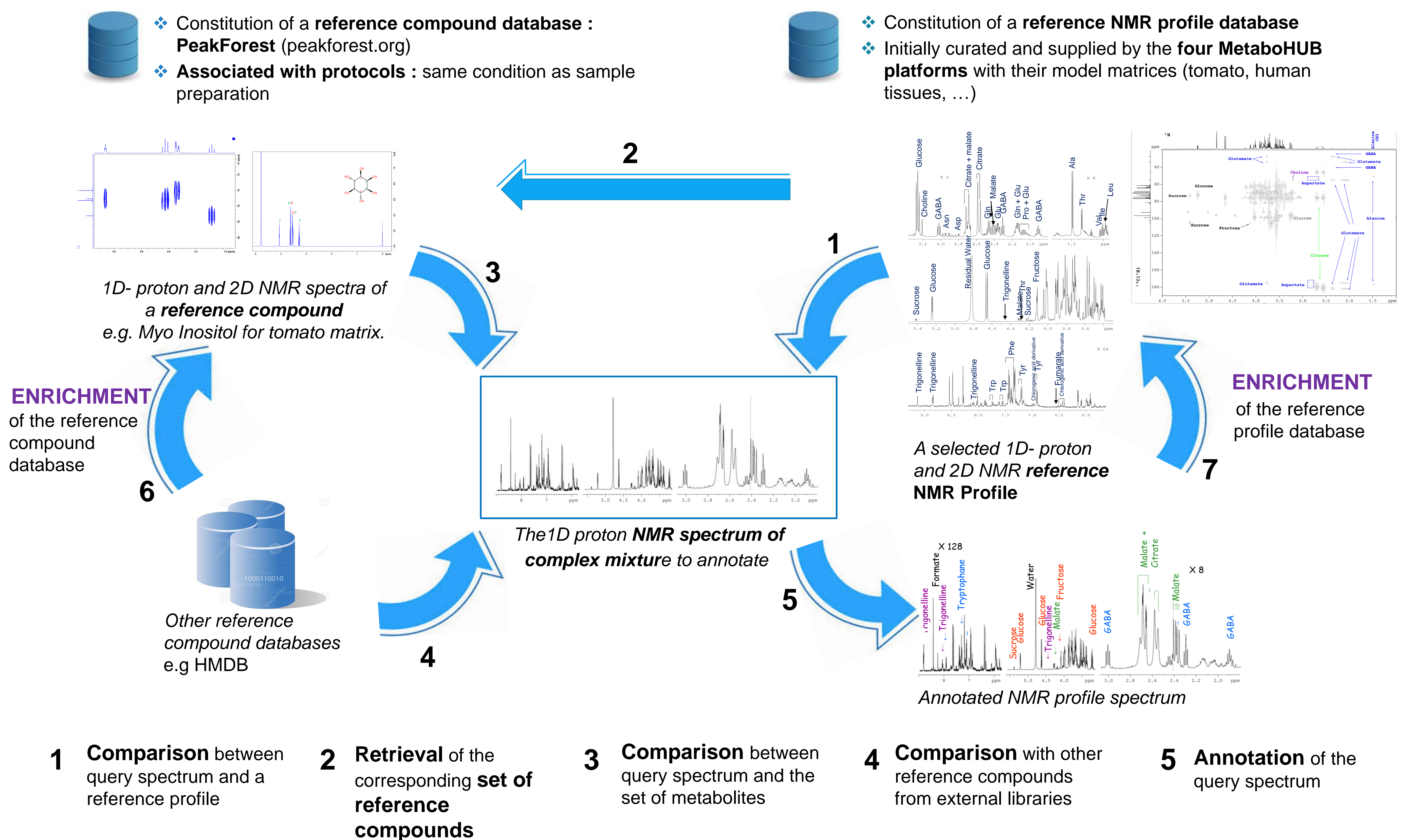
1D proton NMR spectroscopy is largely used to characterize **extracts** or **biofluids for metabolomic analyzes**. A 1D proton NMR spectrum of a complex mixture is a signature or fingerprint resulting from the superposition of the spectra of all the molecules constituting this mixture weighed by their concentrations.

- The **identification of a compound** is sometimes only based on one or two resonances, that cannot be validated without using 2D NMR experiments such as JRES or HSQC to comply with the Metabolomics Standards Initiative guidelines (MSI) on the identification of metabolites^[1, 2].
- **Identification and quantification** of more numerous compounds require a very good knowledge of the composition of the studied matrix.
- **Search for candidate compounds** in a 1D proton-NMR spectra library covering all species and many metabolic pathways provides a very rich but inextricable information without the look of an expert.

Purpose: Annotate a NMR Spectrum of Complex Mixture by relying on a Metabolic Profile

The main strategy is to capitalize on experts' knowledge

for each model matrix defined as a metabolic profile annotated with all the reference compounds of interest



Implementation Roadmap

- ❖ Establish a **library of reference 1D and 2D NMR spectra of interest compounds** constituting each NMR Profile, and acquired in the same conditions of pH and similar ionic strength^[1, 2],
- ❖ Implement "**peak matching**" algorithms^[3] for targeted candidate searching on the library of the corresponding NMR Profile.
- ❖ All the **NMR spectra** of reference compounds and profiles will be modeled, **stored and managed in the "PeakForest database"** (See Poster P1 "PEAKFOREST", Nils Paulhe et al.)

References

Literature cited

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3. Jacob D. et al. An efficient spectra processing method for metabolite identification from 1H-NMR metabolomics data. *Analytical and Bioanalytical Chemistry*, 2013. 405:5049