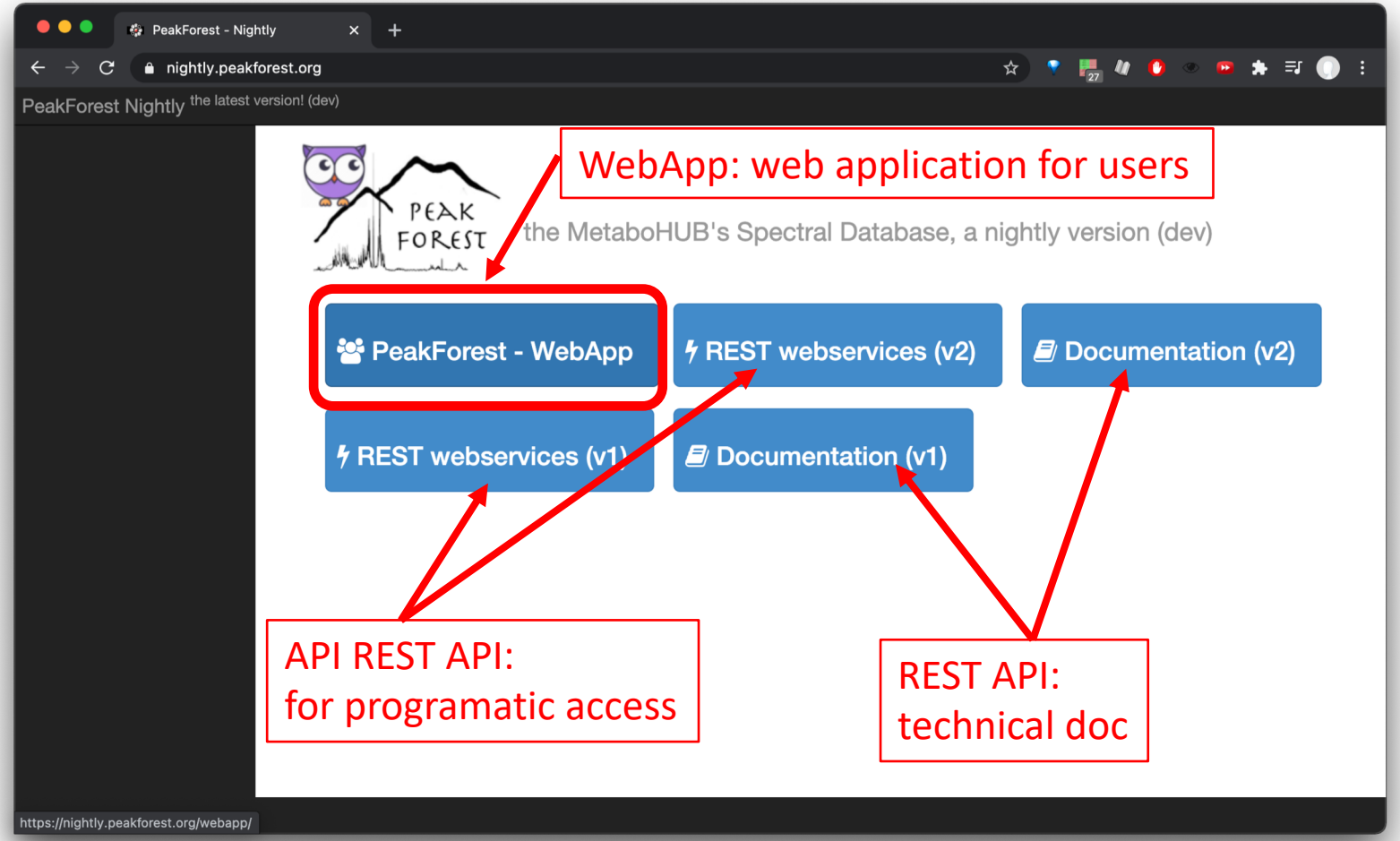
PeakForest HOWTO

Add a NMR spectrum

N. Paulhe - F. Giacomoni

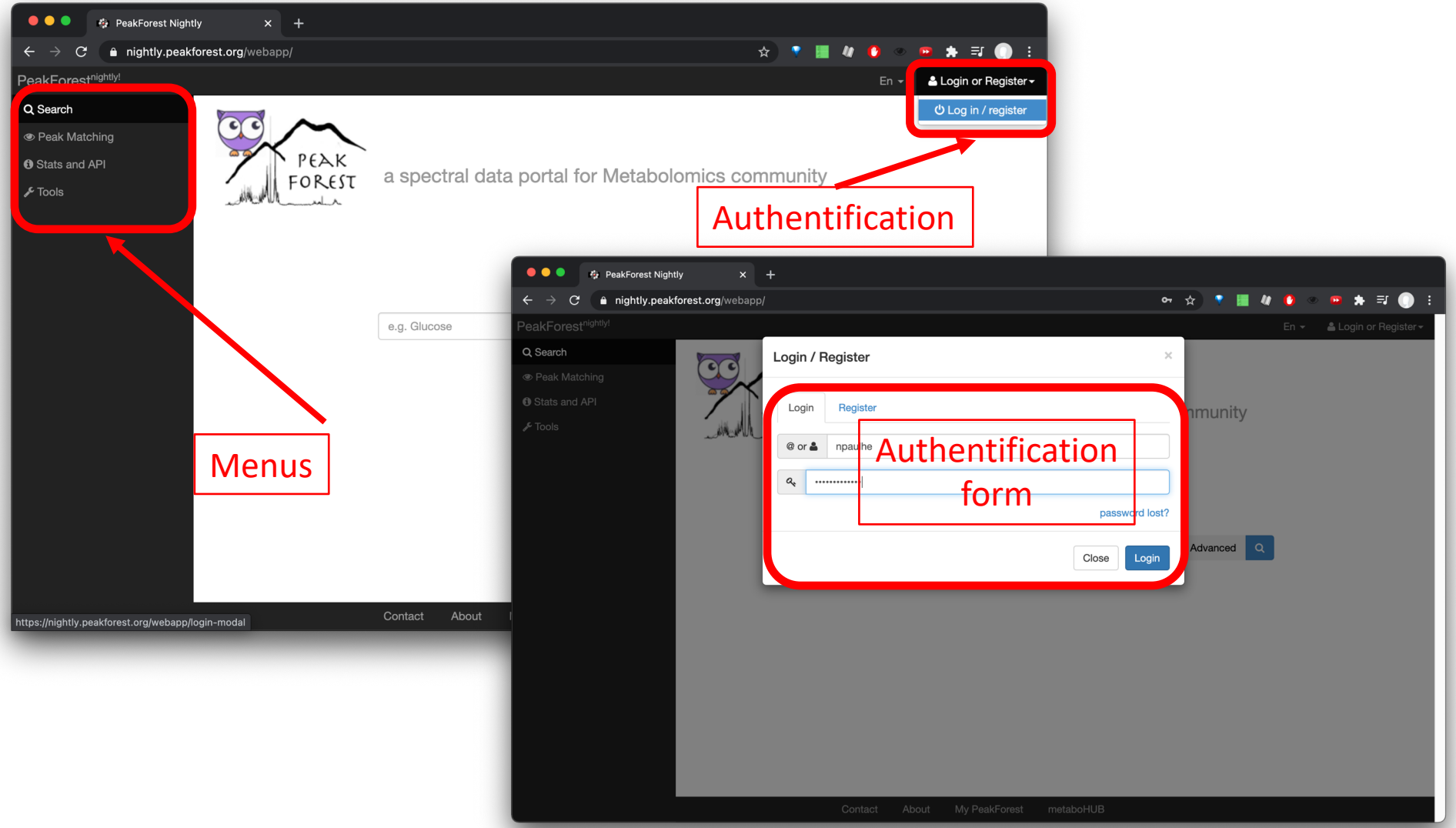
Introduction – PeakForest

Access

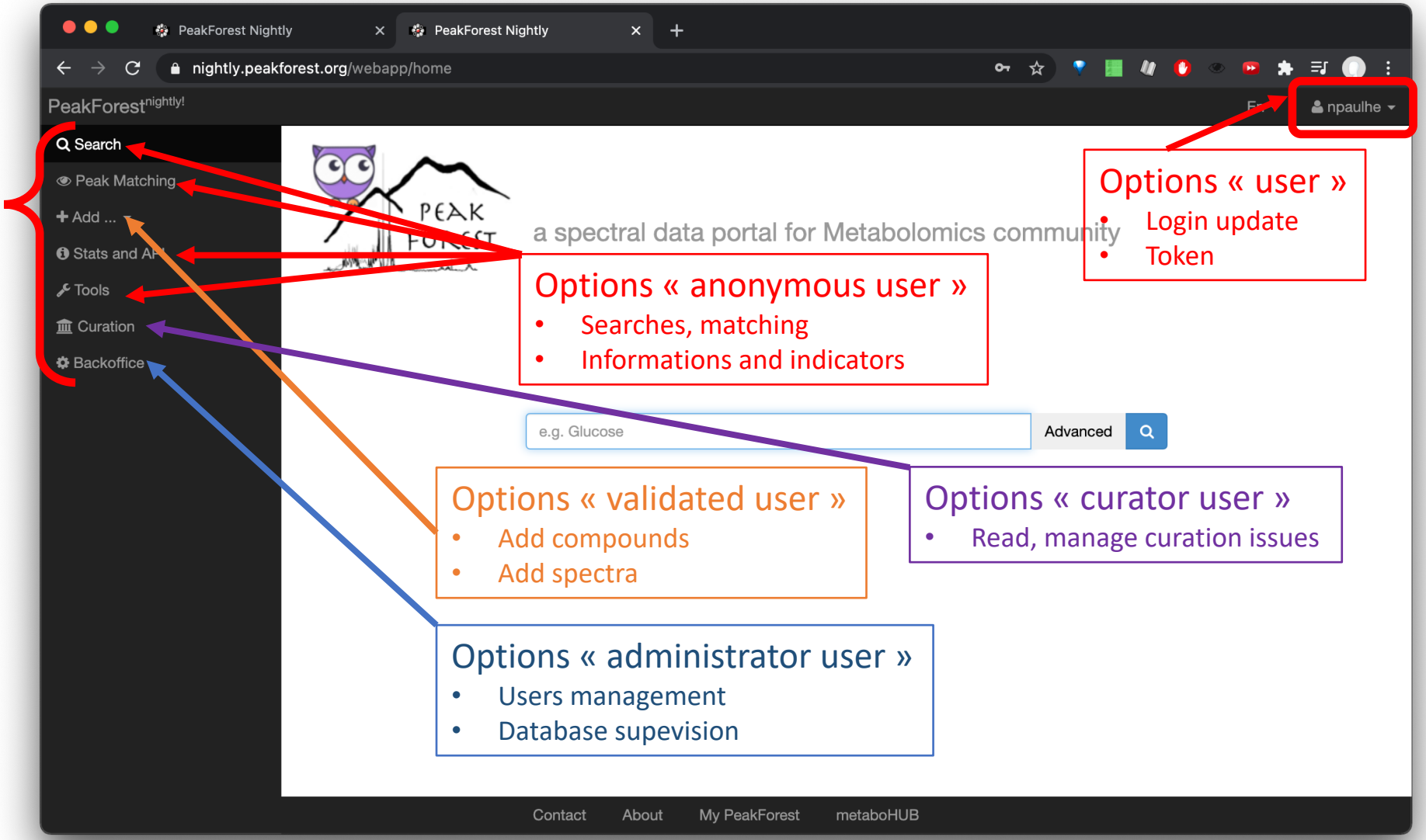


Introduction – PeakForest

Menus and Authentification

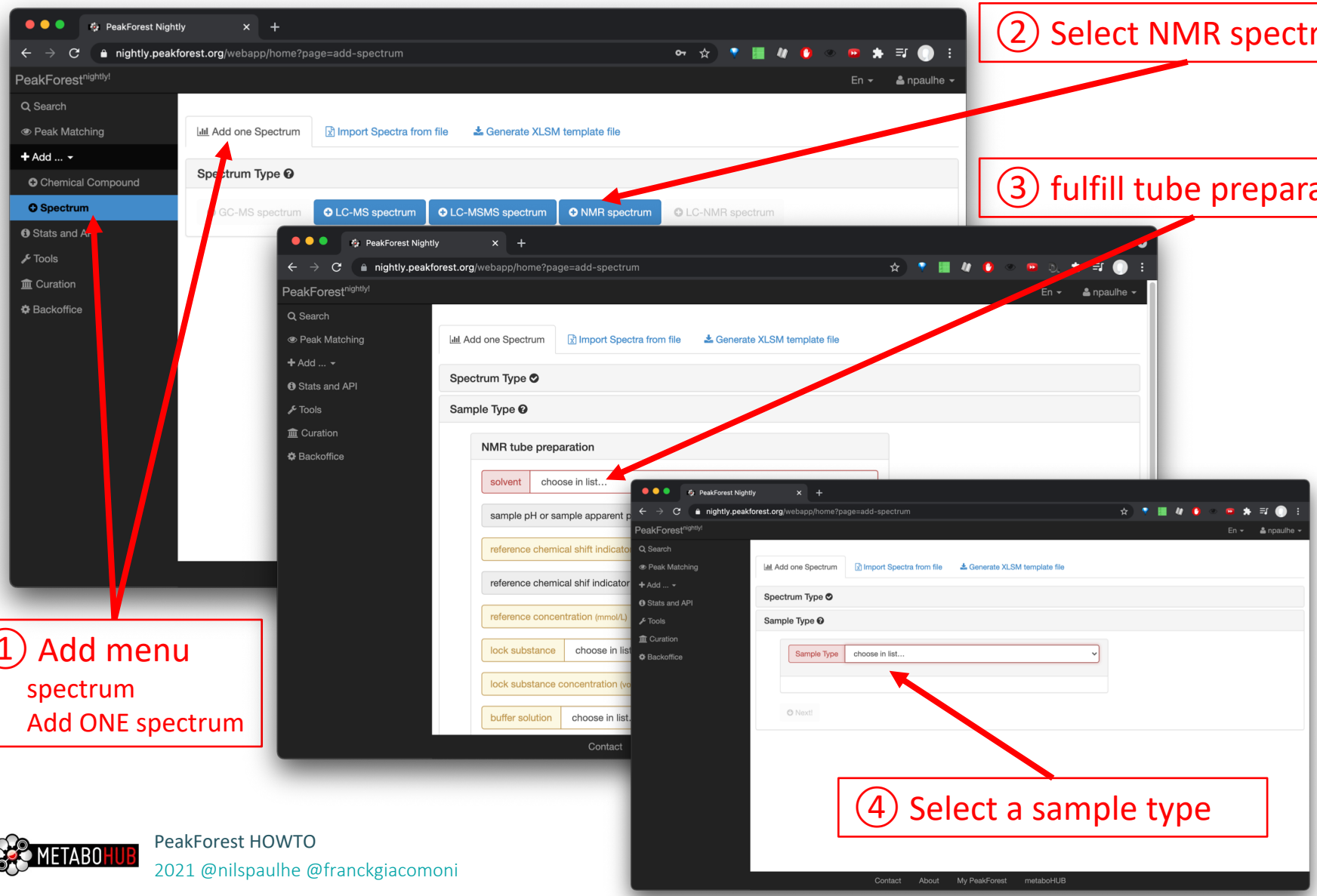


Introduction – PeakForest



Add NMR spectrum

1/5 – Sample and spectral type selection



① Add menu
- spectrum
- Add ONE spectrum

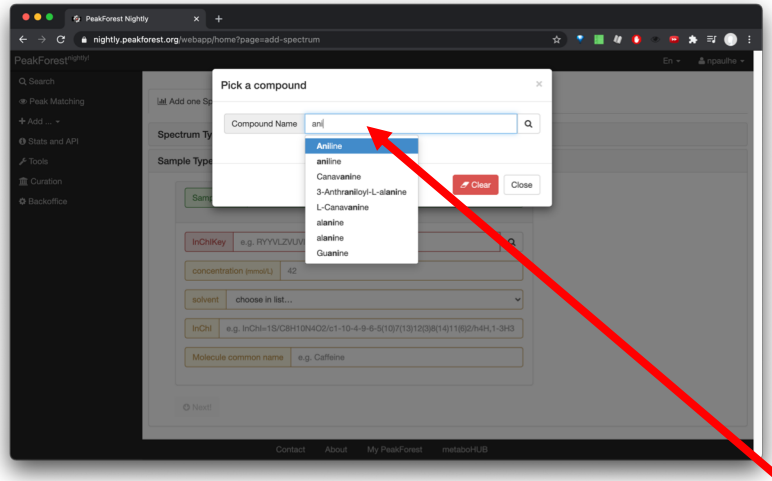
② Select NMR spectrum

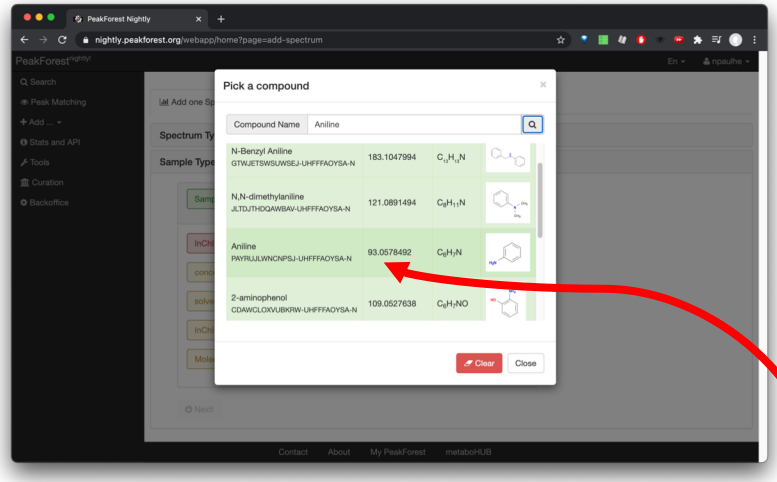
③ fulfill tube preparation

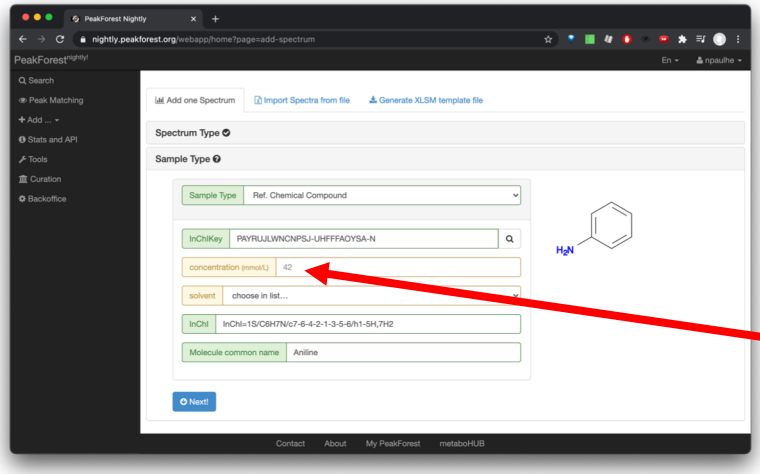
④ Select a sample type

Add a NMR spectrum

2/5 – Sample informations







① Chemical compound search

② compound association

③ Optional metadata

- Solvant
- Concentration
- …

Add a NMR spectrum

3/5 – Analyzer and acquisition metadata

① instrument metadata

② acquisition metadata

③ Optional raw NMR file

- zip
- Brucker file
- Can be link later
- Used for viewer and data extraction

Add a NMR spectrum

4/5 – Peaklists and PeakPatterns informations

① peaklist data

PeakForest Nightly | glycine betaine; 6.0; Proton-1D

nightly.peakforest.org/webapp/home?page=add-spectrum

PeakForest nightly! | En | npaulhe

Search
Peak Matching
Add ...
Stats and API
Tools
Curation
Backoffice

Add one Spectrum | Import Spectra from file | Generate XLSM template file

Spectrum Type
Sample Type
NMR Analyzer
NMR Peaks

② Preview the fingerprint
(will be used in viewer only if no raw data linked)

Peak List | Spectrum Preview

proton nmr peaks

peak index	region	index (F1)	v (F1) [ppm]	v (F1) [Hz]	intensity [abs]	intensity [rel]	half width [ppm]	half width [Hz]	annotation
1			3.9			3.35	0.96		
2			3.27			14.85	0.96		2

This spreadsheet can be fulfilled with a copy/past from brucker software

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Add a NMR spectrum

4/5 – Other informations / validations

① Data checking
- author(s)

② validation
- Import
- Can be exported in a XLSM file

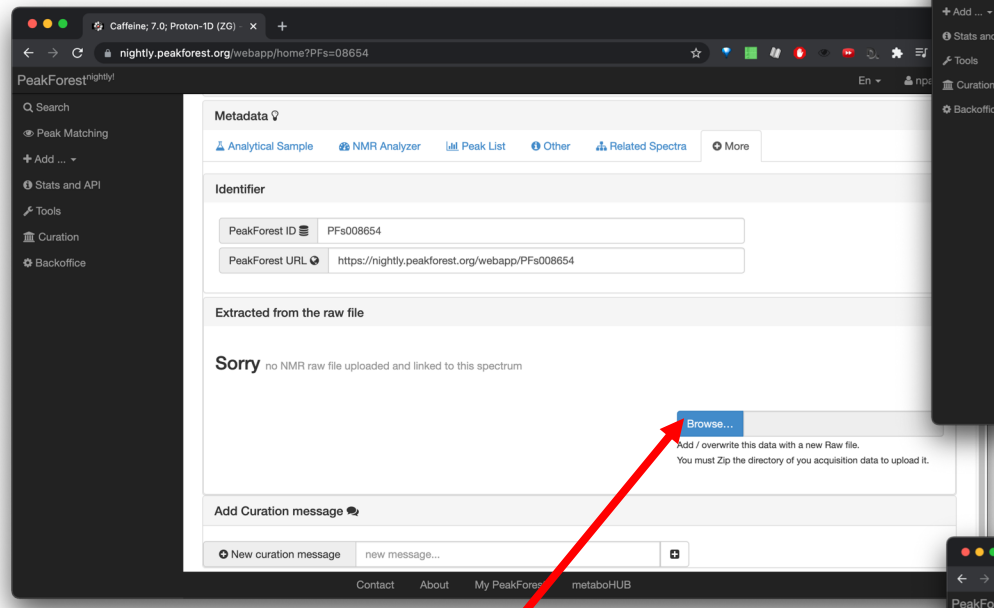
③ add a new acquisition (Cosy/Tocsy/…)

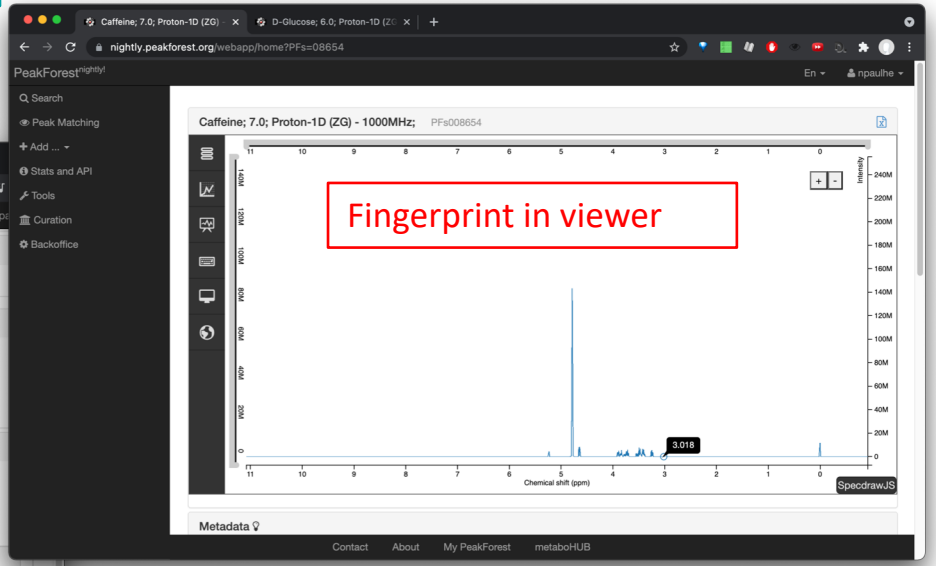
Spectra view and new ID in database

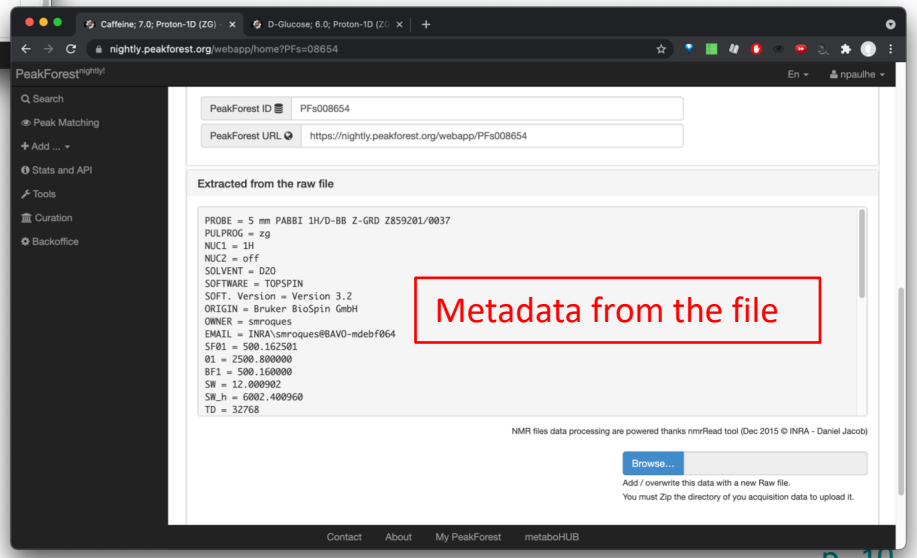
View data/metadata in XLSM format

Add a NMR spectrum

5/5 – add spectrum raw data







① select ZIP with raw NMR data (from brucker)

- If there is a many spectra in the archive, you will be able to select the correct specturm

PeakForest project

contact@peakforest.org