

➤ PeakForest HOWTO

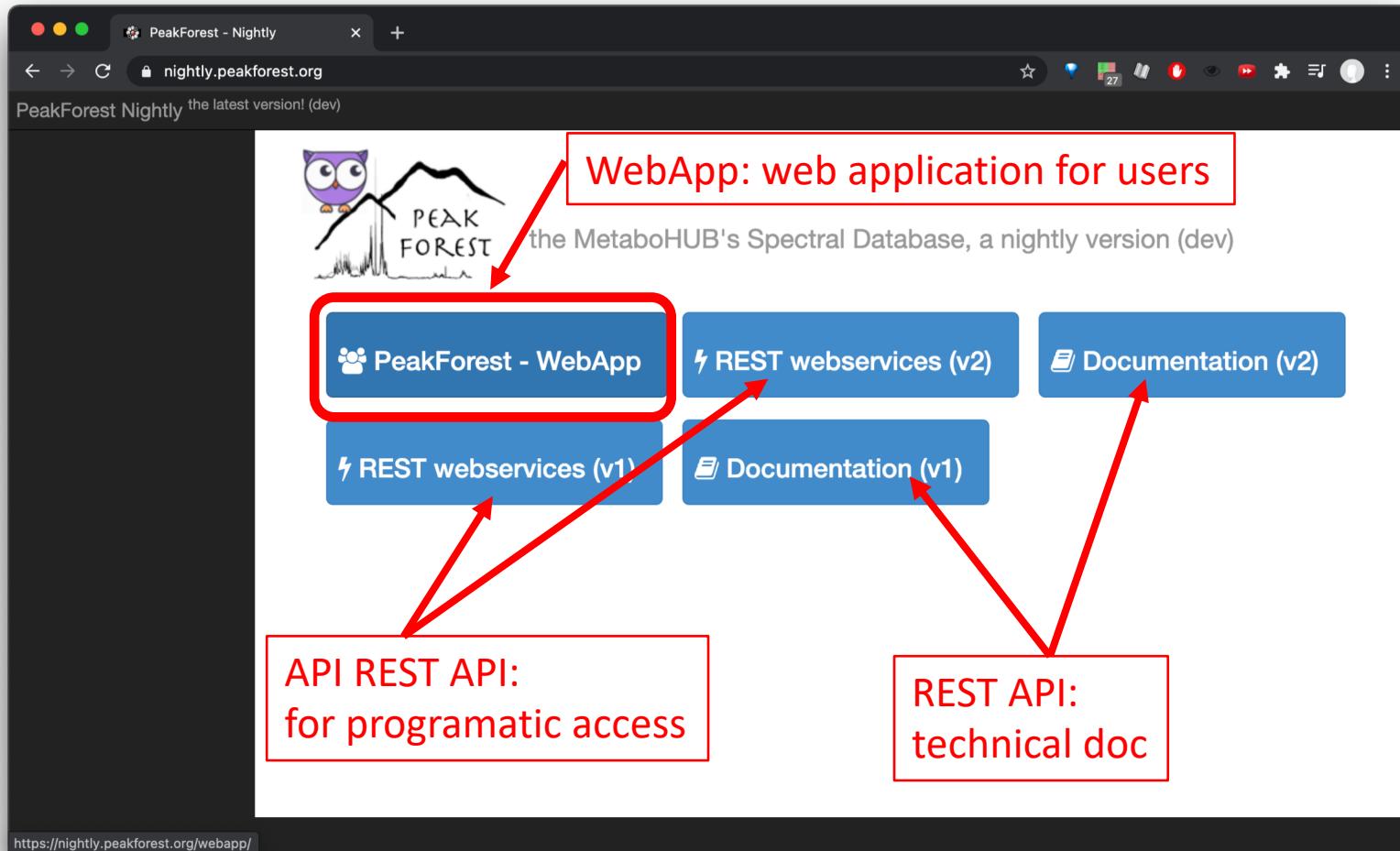
Add a NMR spectrum

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> Introduction – PeakForest

Access



➤ Introduction – PeakForest

Menus and Authentification

The image displays two screenshots of the PeakForest web application interface. The top screenshot shows the main landing page with a navigation bar, a search bar, and a sidebar containing links for 'Search', 'Peak Matching', 'Stats and API', and 'Tools'. A red box highlights the sidebar, and a red arrow labeled 'Menus' points to it. Another red box highlights the 'Login or Register' dropdown menu, and a red arrow labeled 'Authentification' points to the 'Log in / register' option. The bottom screenshot shows a modal window titled 'Login / Register' with tabs for 'Login' and 'Register'. It contains fields for email/username ('@ or & npauhe') and password ('.....'). A red box highlights this modal window, and a red arrow labeled 'Authentification form' points to it.

PeakForest Nightly | https://nightly.peakforest.org/webapp/

PeakForest Nightly | https://nightly.peakforest.org/webapp/login-modal

En | Login or Register | Log in / register

Search

Peak Matching

Stats and API

Tools

a spectral data portal for Metabolomics community

Authentification

e.g. Glucose

Contact About

Log in / register

Login Register

@ or & npauhe

.....

password lost?

Close Login

Contact About My PeakForest metaboHUB

➤ Introduction – PeakForest

The screenshot shows the PeakForest web application interface. On the left, a sidebar menu lists: Search, Peak Matching, Add ..., Stats and API, Tools, Curation, and Backoffice. A central search bar contains the placeholder "e.g. Glucose" and has "Advanced" and search buttons. The main content area features a cartoon owl logo with the text "PEAK FOREST". Below the owl is the tagline "a spectral data portal for Metabolomics community". Four boxes highlight user options:

- Options « anonymous user »**
 - Searches, matching
 - Informations and indicators
- Options « validated user »**
 - Add compounds
 - Add spectra
- Options « curator user »**
 - Read, manage curation issues
- Options « administrator user »**
 - Users management
 - Database supevision

Red arrows point from the sidebar menu items to their corresponding option boxes. A red box highlights the "User" dropdown in the top right corner, which is also pointed to by a red arrow.

> 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

The screenshot shows the 'Add one Spectrum' page. In the 'Sample Type' section, the 'Ref. Chemical Compound' tab is selected. In the 'Compound Name' input field, 'anil' is typed, and a dropdown menu lists several compounds starting with 'anil', including Aniline, aniline, Canavanine, 3-Anthranoyl-L-alanine, L-Caravanine, alanine, alanine, and Quanine. Below the dropdown, there are fields for 'concentration (mmol/L)', 'solvent', and 'InChI'.

The screenshot shows the 'Add one Spectrum' page with the search results for 'Aniline'. The first result is highlighted: 'Aniline' with InChI key 'PAVRULUWCNCNPSJ-UHFFFAOYSA-N', ID '93.0578492', and formula 'C₆H₅N'. Other results listed include 'N,N-dimethylaniline' and '2-aminophenol'.

① Chemical compound search

② compound association

③ Optional metadata

- Solvant
- Concentration
- ...

The screenshot shows the 'Add one Spectrum' page with optional metadata fields. The 'Sample Type' is set to 'Ref. Chemical Compound'. The 'InChIkey' field contains 'PAVRULUWCNCNPSJ-UHFFFAOYSA-N', and the 'concentration (mmol/L)' field contains '42'. A chemical structure of aniline is shown next to the InChIkey. Below these fields are 'solvent', 'InChI', and 'Molecule common name' fields, all containing 'Aniline'. At the bottom is a 'Next!' button.

> Add a NMR spectrum

3/5 – Analyzer and acquisition metadata

The screenshot shows the PeakForest web interface for adding a new NMR spectrum. It consists of three main tabs:

- Instrument**: Contains fields for 'Instrument name' (with a dropdown placeholder 'choose in list...'), 'Magnetic field strength (MHz)', 'Software', 'NMR probe', 'Cell or Tube', 'NMR tube diameter (mm)', and 'Flow cell volume (µl)'. The 'Flow cell volume' field has a placeholder 'e.g. 60'.
- Acquisition**: Contains fields for 'programm' (set to 'Proton acquisition'), 'Pulse sequence' (set to 'PULPROG'), 'Pulse angle (°)' (set to 'F1'), 'Number of points' (set to 'TD'), 'Number of scans' (set to 'NS'), 'Temperature (K)' (set to 'TE'), 'Relaxation delay D1 (s)' (set to 'DS'), and 'SW (ppm)' (set to 'SW').
- Spectra processing parameters**: Contains fields for 'Fourier transform' (placeholder 'choose in list...'), 'SI' (placeholder 'choose in list...'), 'Line broadening' (placeholder 'e.g.: 0.3 Hz'), and a 'Raw spectra file' section with a 'Browse...' button and a note: 'Add a new *Raw* file. You must Zip the directory of your acquisition data to upload it.'

① instrument metadata (red box): Points to the 'Instrument name' field in the first tab.

② acquisition metadata (red box): Points to the 'Flow cell volume (µl)' field in the second tab.

③ Optional raw NMR file (red box): Points to the 'Raw spectra file' section in the third tab.

> Add a NMR spectrum

4/5 – Peaklists and PeakPatterns informations

① peaklist data

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

This spreadsheet can be fulfilled with a copy/paste from bruker software

PeakForest(nightly)

Add one Spectrum Import Spectra from file Generate XLSM template file

Spectrum Type Sample Type NMR Analyzer

Peak List Spectrum Preview

proton nmr peaks

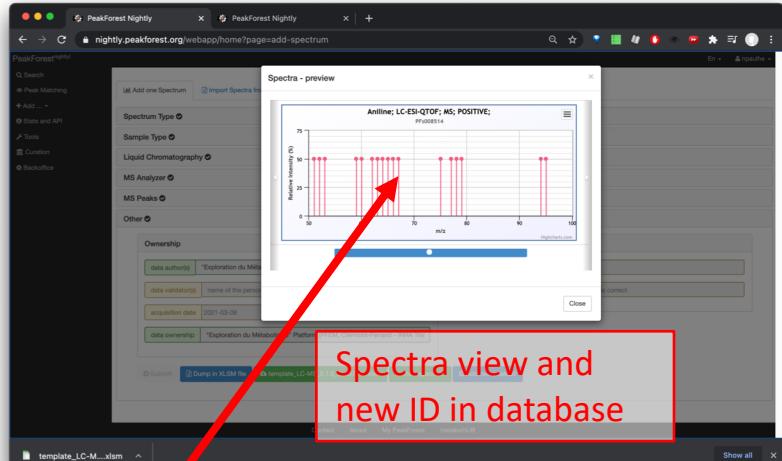
peak index	region	index (F1)	v (F1) [ppm]	v (F1) [Hz]	intensity [abs]	intensity [rel]	half width [ppm]	half width [Hz]	annotation
1			3.9		3.35	0.96			
2			3.27		14.85	0.96			2

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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/...)

m/z	absolute intensity	relative intensity (%)	theo. mass	delta (ppm)	RDB equiv	composition	attribution	identification level
11	51.029293	50	0	0	0	[CH3N]	[MH-H]·CH3N+	Confident identification
12	52.031296	50	0	0	0	[CH3N]	NA	Confident identification
13	53.026545	50	0	0	0	[CH3]	NA	Confident identification
14	54.027269	50	0	0	0	[CH3]2	[MH-H]2N+(NH)2	Confident identification
15	60.012024	50	0	0	0	[2H3]	[MH-H]2N+(NH)2	Confident identification
16	62.038907	50	0	0	0	[OB(OH)]	[MH-H]·CH3O+	Confident identification
17	63.029293	50	0	0	0	[O(SN)]	[MH-H]·CH3N+	Confident identification
18	64.031817	50	0	0	0	[CH6]	[MH-H]2O+	Confident identification

View data/metadata in XLSM format
p. 9

> 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

Fingerprint in viewer

Metadata from the file

PeakForest HOWTO
2021 @nilspaulhe @franckgiacomoni

PeakForest ID: PFs008654
PeakForest URL: https://nightly.peakforest.org/webapp/PFs008654

Extracted from the raw file

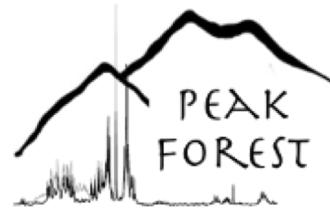
```
PROBE = 5 mm PABBI 1H/D-BB Z-GRD Z859201/0037
PULPROG = zg
NUC1 = 1H
NUC2 = 13C
SOLVENT = D2O
SOFTWARE = TOPSPIN
SOFT, Version = Version 3.2
ORIGIN = Bruker BioSpin GmbH
OWNER = smroques
EMAIL = INRA.smroques@BAV0-mdeb064
SF01 = 500.162501
01 = 2500.800000
BF1 = 50.160000
SW = 12.000902
SW_h = 6002.400960
TD = 32768
```

NMR files data processing are powered thanks nmrRead tool (Dec 2015 © INRA - Daniel Jacob)

Browse...
Add / overwrite this data with a new Raw file.
You must Zip the directory of your acquisition data to upload it.



PeakForest project



contact@peakforest.org

