

## ➤ PeakForest HOWTO

Add a LC/MS spectrum

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# ➤ Introduction – PeakForest

## Access

The screenshot shows the PeakForest website interface. At the top, the browser address bar displays `nightly.peakforest.org`. The page header includes the PeakForest logo (an owl) and the text "PEAK FOREST the MetaboHUB's Spectral Database, a nightly version (dev)".

The main content area features a navigation menu with five items, each in a blue box:

- PeakForest - WebApp (highlighted with a red box)
- REST webservice (v2)
- Documentation (v2)
- REST webservice (v1)
- Documentation (v1)

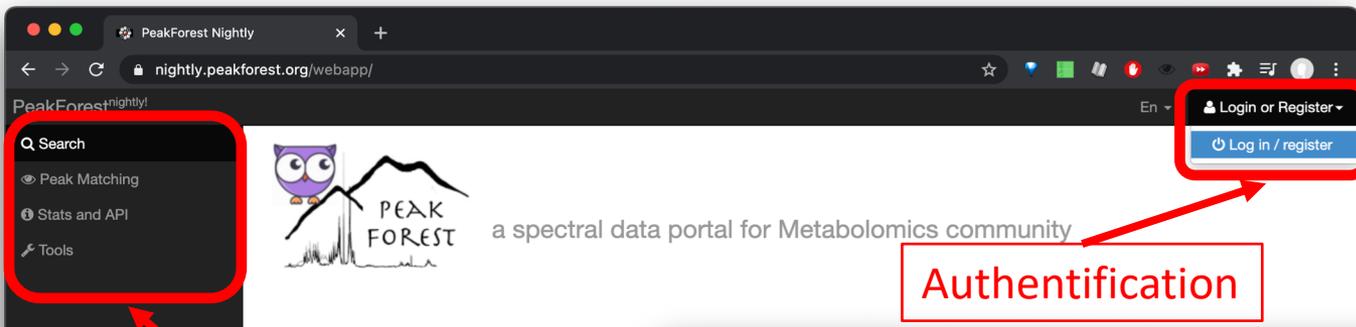
Red arrows and boxes provide additional context:

- A red box at the top right contains the text "WebApp: web application for users", with an arrow pointing to the "PeakForest - WebApp" button.
- A red box at the bottom left contains the text "API REST API: for programatic access", with arrows pointing to the "REST webservice (v1)" and "REST webservice (v2)" buttons.
- A red box at the bottom right contains the text "REST API: technical doc", with arrows pointing to the "Documentation (v1)" and "Documentation (v2)" buttons.

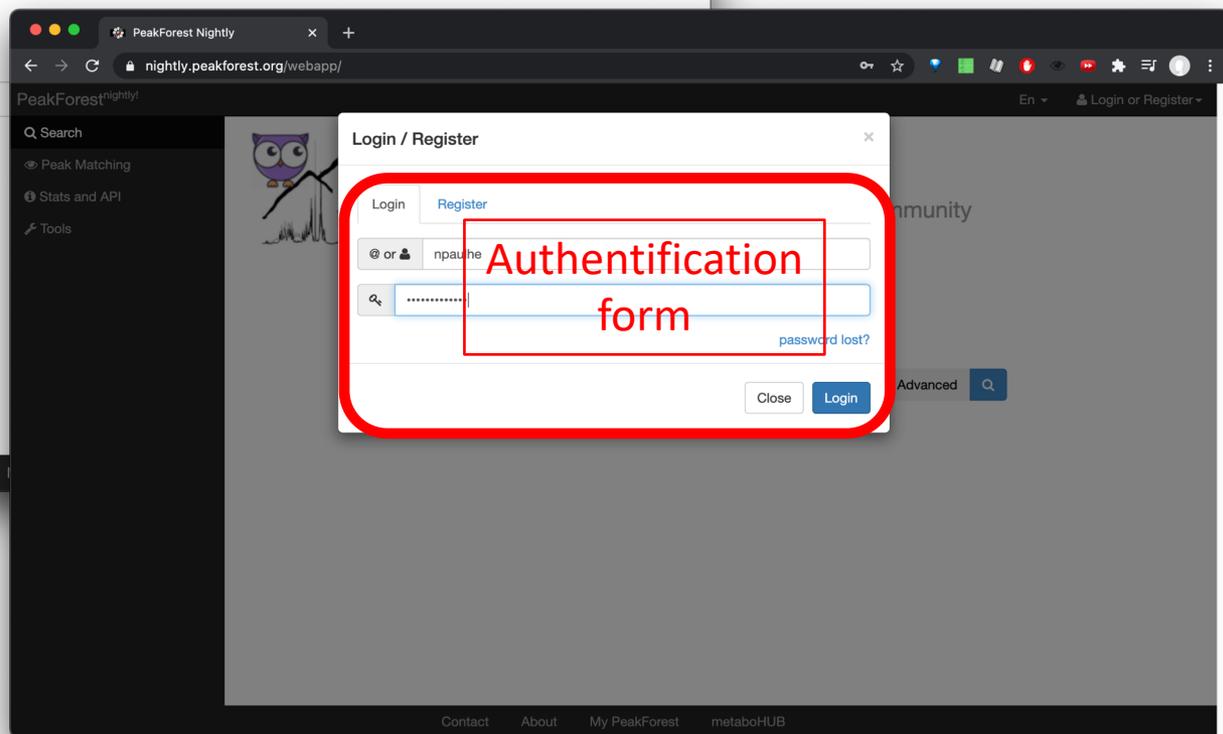
The browser's address bar at the bottom shows the URL `https://nightly.peakforest.org/webapp/`.

# ➤ Introduction – PeakForest

## Menus and Authentication



Menus



# ➤ Introduction – PeakForest

The screenshot shows the PeakForest Nightly web application interface. The browser address bar displays `nightly.peakforest.org/webapp/home`. The page header includes the PeakForest logo and the text "a spectral data portal for Metabolomics community". A search bar contains the text "e.g. Glucose" and an "Advanced" search button. A navigation menu on the left lists: Search, Peak Matching, Add ..., Stats and AP, Tools, Curation, and Backoffice. A user profile dropdown in the top right shows the name "npaulhe".

**Options « user »**

- Login update
- Token

**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 supervision

# ➤ Add a LC/MS spectrum

## 1/7 – Sample and spectral type selection

PeakForest Nightly

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

PeakForest<sup>nightly!</sup>

Q Search

Peak Matching

+ Add ...

Chemical Compound

Spectrum

Stats and API

Tools

Curation

Backoffice

Add one Spectrum

Import Spectra from file

Generate XLSM template file

Spectrum Type

GC-MS spectrum

LC-MS spectrum

LC-MSMS spectrum

NMR spectrum

LC-NMR spectrum

② Select LCMS spectra

③ Select a sample type

① Add menu

- spectrum
- Add ONE spectrum

PeakForest Nightly

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

PeakForest<sup>nightly!</sup>

Q 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

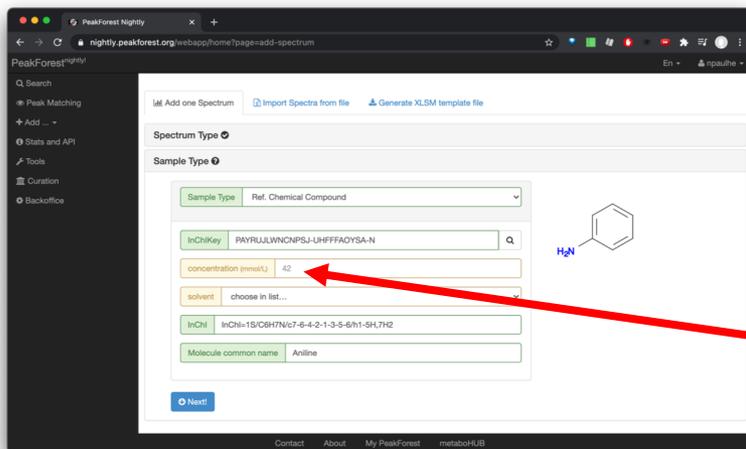
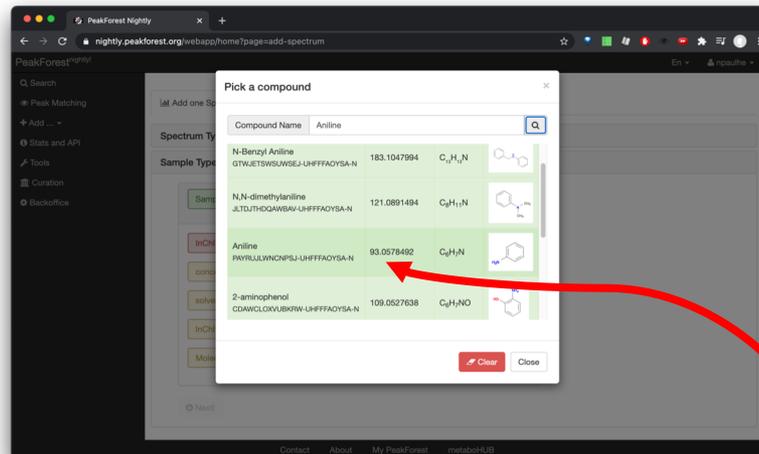
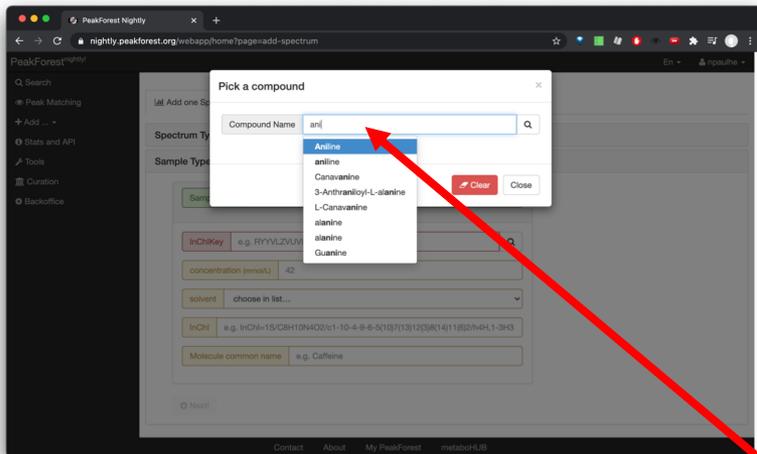
Sample Type choose in list...

Next!

Contact About My PeakForest metaboHUB

# ➤ Add a LC/MS spectrum

2/7 – Sample information



① Chemical compound search

② Compound association

③ Optional metadata

- Solvent
- Concentration
- ...

# ➤ Add a LC/MS spectrum

## 3/7 – Chromatographic metadata

### ① Method selection

- Informations can be prefilled (Cf dedicated technical doc)

### ② Fill or update metadata values

### ③ next!

Method selection

- Informations can be prefilled (Cf dedicated technical doc)

Fill or update metadata values

next!

# ➤ Add a LC/MS spectrum

## 4/7 – Analyser metadata

The screenshot shows the 'Add Spectrum' form in the PeakForest web application. The form is divided into several sections: 'Spectrum Type', 'Sample Type', 'Liquid Chromatography', and 'MS Analyzer'. The 'MS Analyzer' section is further divided into 'Analyzer' and 'Molecule Ionization'.

**Annotations:**

- A red box with the text "① Fill or update metadata values" is positioned above the 'Molecule Ionization' section. A red arrow points from this box to the 'Ionization method (POS/NEG)' dropdown menu.
- A red box with the text "② next!" is positioned above the 'Next!' button. A red arrow points from this box to the 'Next!' button.

**Form Fields:**

- Spectrum Type:** Add one Spectrum, Import Spectra from file, Generate XLSM template file
- Sample Type:** [Dropdown]
- Liquid Chromatography:** [Dropdown]
- MS Analyzer:**
  - Analyzer:**
    - Instrument: Q-TOF
    - Model: QToF micro (Micromass Waters)
    - Ion analyzer Type: QTOF
  - Molecule Ionization:**
    - Ionization method (POS/NEG): ESI
    - Spray (needle) gas flow (arbitrary in Xcalibur, POS/NEG): 40
    - Vaporizer gas flow (arbitrary in Xcalibur, POS/NEG): e.g. 10 (POS), e.g. 5 (NEG)
    - Vaporizer temperature (°C, POS/NEG): 200
    - Source gas flow (arbitrary in Xcalibur, POS/NEG): 9
    - Ion transfer tube temperature / Transfer capillary temperature (°C, POS/NEG): e.g. 350 (POS), e.g. 350 (NEG)
    - High voltage (ESI) / Corona voltage (APCI) (in kV, POS/NEG): 2.5

**Buttons:** Add one Spectrum, Import Spectra from file, Generate XLSM template file, Next!

# ➤ Add a LC/MS spectrum

## 5/7 – Peaklist information

The screenshot shows the 'MS Analyzer' interface with the 'MS Peaks' section. The table below lists the peak data:

| m/z     | absolute intensity | relative intensity (%) | theo. mass | delta (ppm) | RDB Equiv. | composition | attribution    |
|---------|--------------------|------------------------|------------|-------------|------------|-------------|----------------|
| 51.0229 | 50.00              | 50.00                  | 50.000     | 0.0000      |            | -C2H6N      | [M+H-C2H6N]+   |
| 52.0313 | 50.00              | 50.00                  | 0.0000     |             |            | -C2H6N      | NA             |
| 53.0285 | 50.00              | 50.00                  | 0.0000     |             |            | -C2H6       | NA             |
| 59.0280 | 50.00              | 50.00                  | 0.0000     |             |            | -H2C-NH2    | [M+H-H2O-NH2]+ |
| 60.0120 | 50.00              | 50.00                  | 0.0000     |             |            | -NH3        | [M+H-2NH3]+    |
| 62.0389 | 50.00              | 50.00                  | 0.0000     |             |            | -CH3OH      | [M+H-CH3OH]+   |
| 63.0229 | 50.00              | 50.00                  | 0.0000     |             |            | -CH6N       | [M+H-CH6N]+    |
| 64.0182 | 50.00              | 50.00                  | 0.0000     |             |            | -C2H6       | [M+H-C2H6]+    |
| 65.0285 | 50.00              | 50.00                  | 0.0000     |             |            | -C2H5       | NA             |
| 66.0338 | 50.00              | 50.00                  | 0.0000     |             |            | -C2H5       | [M+H-C2H5]+    |
| 67.0422 | 50.00              | 50.00                  | 0.0000     |             |            | -C2H3       | NA             |
| 75.0229 | 50.00              | 50.00                  | 0.0000     |             |            | -H2-NH3     | [M+H-H2-NH3]+  |
| 77.0286 | 50.00              | 50.00                  | 0.0000     |             |            | -NH3        | [M+H-NH3]+     |
| 78.0338 | 50.00              | 50.00                  | 0.0000     |             |            | -CH4        | [M+H-CH4]+     |
| 79.0422 | 50.00              | 50.00                  | 0.0000     |             |            | -CH3        | NA             |
| 94.0651 | 50.00              | 50.00                  | 0.0000     |             |            | +H          | [M+H]+         |
| 95.0622 | 50.00              | 50.00                  | 0.0000     |             |            | 15N         | [M+H-15N]      |

- ① Peaklist data
  - MZ range
  - Polarity / Resolution
  - Peaklist + attributions

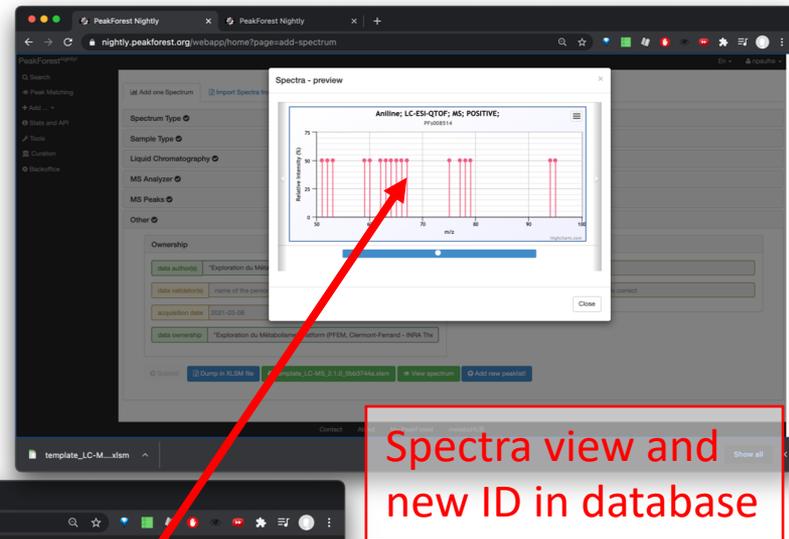
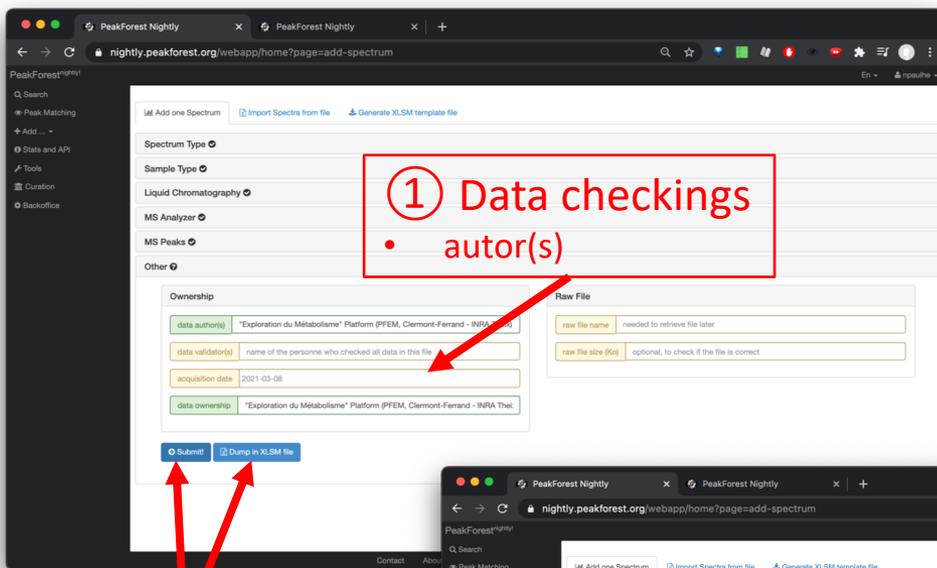
- ② Peaklist checkings and visualization

- ③ next!

The screenshot shows the 'MS Analyzer' interface with the 'Spectrum Preview' section. The plot displays relative intensity versus m/z, with several peaks highlighted in red. The x-axis ranges from 50 to 110 m/z, and the y-axis ranges from 0 to 60 relative intensity.

# ➤ Add a LC/MS spectrum

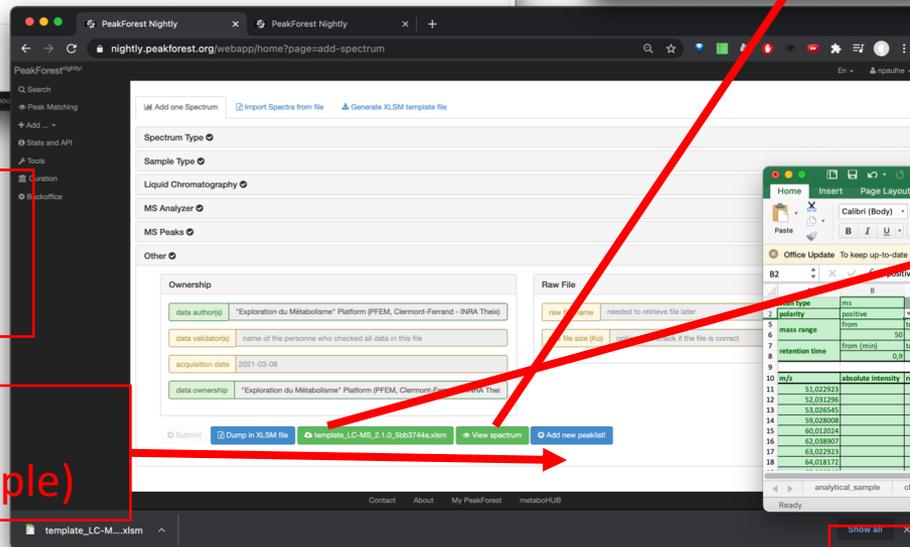
## 6/7 – Other information / validation



**2 Validation**

- Import
- Possible Export in XLSM file

**3 Add a new peaklist (Negative mode for example)**



| Retention time | mass range | absolute intensity | relative intensity (%) | thres. mass | delta (ppm) | RDB equiv. | composition | attribution        | identification level |
|----------------|------------|--------------------|------------------------|-------------|-------------|------------|-------------|--------------------|----------------------|
| 51.022923      | 50         | 50                 | 0                      | 0           | 0           | 0          | -(CH2N)     | [(M+H)-CH2N+]      | Confident identifi   |
| 52.031296      | 50         | 0                  | 0                      | 0           | 0           | 0          | -(CH2N)     | NA                 | Confident identifi   |
| 53.029544      | 50         | 0                  | 0                      | 0           | 0           | 0          | -(CH2S)     | NA                 | Confident identifi   |
| 59.028008      | 50         | 0                  | 0                      | 0           | 0           | 0          | -(H2O)-2NH2 | [(M+H)-(H2O)-2NH3] | Confident identifi   |
| 60.022034      | 50         | 0                  | 0                      | 0           | 0           | 0          | -(NH2)      | [(M+H)-2NH3]       | Confident identifi   |
| 62.028907      | 50         | 0                  | 0                      | 0           | 0           | 0          | -(CH2O)     | [(M+H)-CH2O]       | Confident identifi   |
| 63.022923      | 50         | 0                  | 0                      | 0           | 0           | 0          | -(CH2S)     | [(M+H)-CH2S]       | Confident identifi   |
| 64.028912      | 50         | 0                  | 0                      | 0           | 0           | 0          | -(CH2H)     | [(M+H)-CH2H]       | Confident identifi   |

**View data/metadata in XLSM format**



# PeakForest project



[contact@peakforest.org](mailto:contact@peakforest.org)

