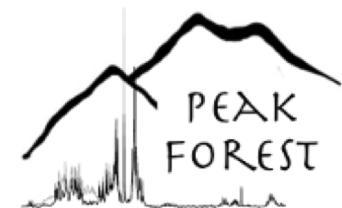


➤ PeakForest HOWTO

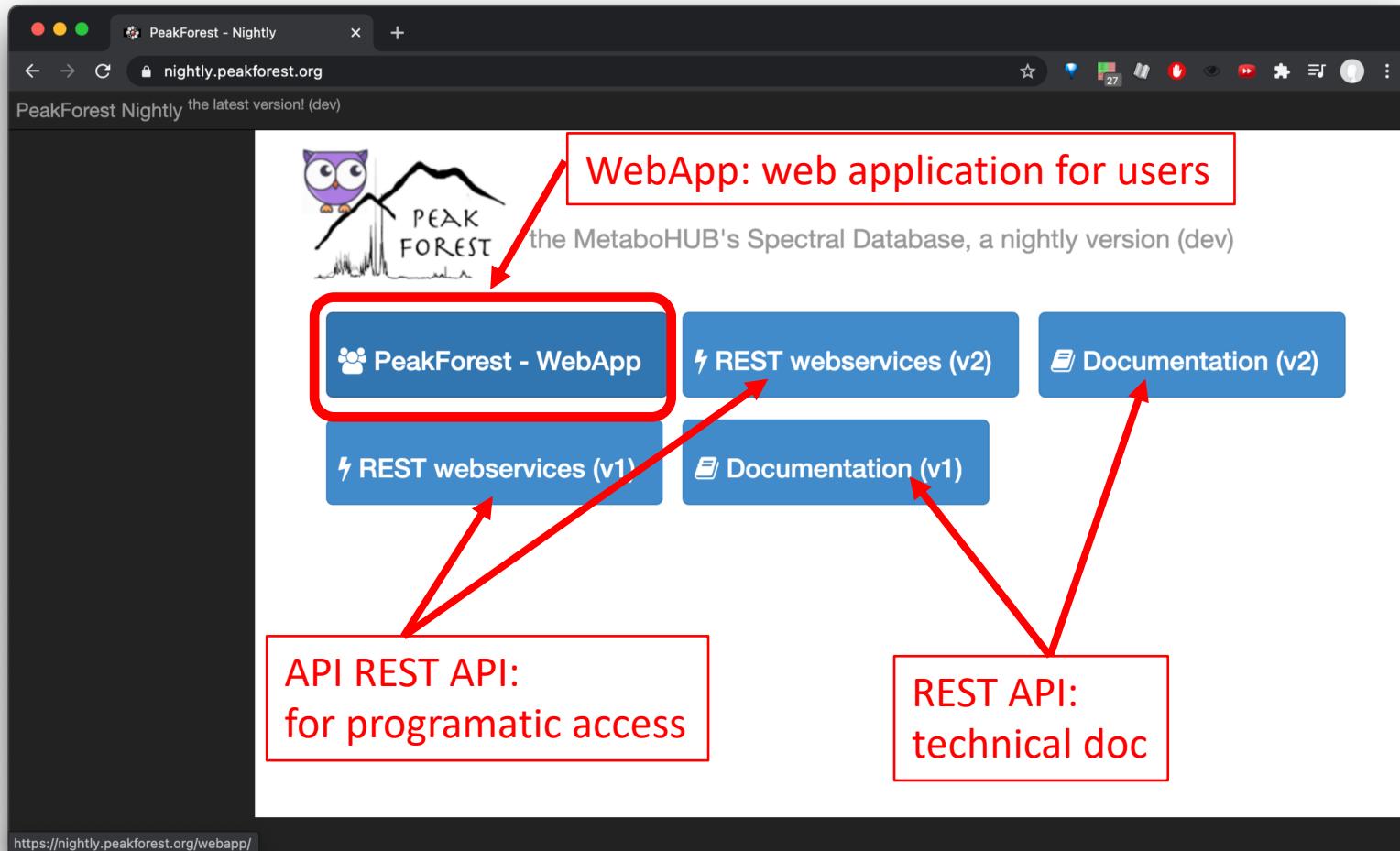
Data curation

N. Paulhe - F. Giacomoni



➤ 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 'Search', 'Peak Matching', 'Stats and API', and 'Tools'. A red box highlights the sidebar with the label 'Menus' below it. 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 with the label 'Authentification form' below it. Red arrows point from the 'Menus' label to the sidebar and from the 'Authentification' label to the modal window.

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

PeakForest Nightly! a spectral data portal for Metabolomics community

En ▾ Login or Register ▾ Log in / register

Search

Peak Matching

Stats and API

Tools

e.g. Glucose

Authentification

Authentification form

Contact About

https://nightly.peakforest.org/webapp/login-modal

Contact About My PeakForest metaboHUB

➤ Introduction – PeakForest

The screenshot shows the PeakForest web application interface. On the left, a sidebar lists navigation items: Search, Peak Matching, Add ..., Stats and API, Tools, Curation, and Backoffice. A central search bar contains the placeholder "e.g. Glucose" and includes Advanced and search buttons. The main content area features a cartoon owl logo with the text "PEAK FOREST". A banner below the logo reads "a spectral data portal for Metabolomics community". To the right, a user profile dropdown menu is open, showing the username "npaulhe". Red arrows point from the sidebar items to four callout boxes: "Options « anonymous user »" (red border), "Options « validated user »" (orange border), "Options « curator user »" (purple border), and "Options « administrator user »" (blue border). Each callout box lists specific permissions or tasks.

- 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

➤ Data curation – Add an issue

1/2 – Spectra card access

The screenshot shows two windows of the PeakForest software interface. The left window displays a mass spectrum plot titled "Aniline; LC-ESI-Q-TOF; MS; POSITIVE; PFs08515". The x-axis is labeled "m/z" and ranges from 50 to 100. The y-axis is labeled "Relative Intensity (%)" and ranges from 0 to 60. Several peaks are visible, with arrows pointing to specific peaks at m/z values around 53, 55, 60, 65, and 70. Below the plot is a "Metadata" section. The right window shows the same mass spectrum and includes a "Curation" section highlighted with a red box. A red arrow points from the "Add Curation message" input field in the curation section to the "Curation section" label. The curation section contains the following information:

- Compound Name: Aniline
- Formula: C₆H₅N
- Solvent: none
- InChI: InChI=1S/C6H5N/c7-6-4-2-1-3-5-6/h1-5H,7H2
- InChIKey: PwRUJLWNCPNSJ-UHFFFAOYSA-N
- Average Mass: 93.12648 Da

Below the curation section is an "Add Curation message" input field containing the text "erreur annotation peak m/z=53.04". At the bottom of the right window are buttons for "Cancel", "Save Changes", and "Edit".

➤ Data curation – Add an issue

2/2 – write and save the message

The figure consists of three screenshots of the PeakForest web application interface, illustrating the process of adding a curation message.

- Screenshot 1:** Shows the main metadata page for Aniline. A red box highlights the "Compound Name: Aniline" field, which contains "Aniline". A red arrow points from this box to the "Add Curation message" section below. The message input field contains "erreur annotation peak m/z=53.04". A red circle labeled "① write and validate the message" is positioned above the message input field.
- Screenshot 2:** Shows the same metadata page after saving changes. The "Compound Name" field now shows "Aniline" with a blue border. A red box highlights the "Add Curation message" section, which now contains "new message...". A red circle labeled "② save modifications" is positioned above the message input field.
- Screenshot 3:** Shows the same metadata page after saving changes again. The "Compound Name" field now shows "Aniline" with a blue border. The "Add Curation message" section now contains "erreur annotation peak m/z=53.04" and "new message...". A red circle labeled "③ the new message is now visible" is positioned above the message input field.

➤ Data curation – Manage issues

1/2 – Curation interface access

The screenshot shows the PeakForest web application interface. The left sidebar has a dark theme with various menu items: Q. Search, Peak Matching, Add ..., Stats and API, Tools, Curation (which is highlighted in red), and Backoffice. The main content area has a light background. At the top, there are tabs for 'Curation Messages' (highlighted in red), 'Bibliography Annotations', and 'CAS / IUPAC conv.'. Below the tabs is a search bar with placeholder 'e.g. bad kegg id', a dropdown for 'Only waiting' or 'All types', and a magnifying glass icon. The main table lists several entries, each with a yellow background row. The columns are: Message (e.g., 'deux fois le même spectre ajouté en mode positif'), Login (alyssa.bouville@inra.fr), Date (2015/12/16), Status (green circle), Show/Edit entity (blue pencil icon), and Delete message (red trash bin icon). A red arrow points from the 'Curation' menu in the sidebar to the 'Curation Messages' tab in the header.

① Go to the « curation » menu and select « curation messages »

The screenshot shows the PeakForest web application interface. The left sidebar has a dark theme with various menu items: Q. Search, Peak Matching, Add ..., Stats and API, Tools, Curation (which is highlighted in red), and Backoffice. The main content area has a light background. At the top, there are tabs for 'Curation Messages', 'Bibliography Annotations', and 'CAS / IUPAC conv.'. Below the tabs is a search bar with placeholder 'cpd id' and 'cpd name'. The main table lists compound details, each with a blue edit icon. The columns are: cpd id, cpd name, action(s), and edit. The table includes rows for PFc001027 (Chenodeoxycholic Acid), PFc001040 (sinapic acid), PFc001120 (Folic Acid), PFc001130 (D-Glucose 6-phosphate), PFc001155 (dAMP), PFc001189 (Caffeic acid), PFc001191 (Indoleacrylic acid), PFc001193 (Choline), PFc001227 (D-Limonene), and PFc001238 (dUMP). A red box highlights the 'Automatic curation:' section at the bottom of the table, which contains two bullet points: 'Convert compound name into IUPAC name' and 'Convert compound name into CAS'. A red arrow points from the 'Curation' menu in the sidebar to the 'Automatic curation:' section.



➤ Data curation – Manage issues

2/2 – Spectra curation

① Direct acces to data/metadata from the curation message

② Changing for exemple peak attribution information

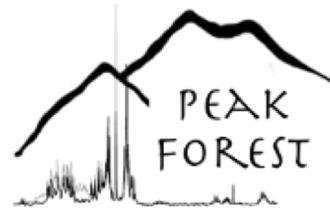
③ save and update message status

Aniline; LC-ESI-Q-TOF; MS; POSITIVE;

m/z	Ri (%)	Theo. Mass	Delta ppm	composition	attribution
51.0229	50.0000	0.0000	0.0000	-C2H5N	[M+H]-C2H5N+
52.0313	50.0000	0.0000	0.0000	-C2H4N	NA
53.0265	50.0000	0.0000	0.0000	(C3H5)	XXX
59.0280	50.0000	0.0000	0.0000	(H2O)-(NH2)	[H+]-[H2O]-(NH3)+
60.0120	50.0000	0.0000	0.0000	-2RN3	[M+H]-2RN3]+
62.0389	50.0000	0.0000	0.0000	-CH3O	[M+H]-CH3OH+
63.0229	50.0000	0.0000	0.0000	-C2H6N	[M+H]-C2H5N+
64.0182	50.0000	0.0000	0.0000	-C2H6	[M+H]-C2H6+
65.0265	50.0000	0.0000	0.0000	(C2H5)	NA
66.0358	50.0000	0.0000	0.0000	-C2H4	[M+H]-C2H4+
67.0424	50.0000	0.0000	0.0000	-C2H5	NA
68.0242	50.0000	0.0000	0.0000	-NH3	[M+H]-H2-(NH3)-
71.0386	50.0000	0.0000	0.0000	-NH3	[M+H]-NH3+
73.0505	50.0000	0.0000	0.0000	-CH4	[M+H]-CH4+
74.0446	50.0000	0.0000	0.0000	-CH3	NA
75.0651	50.0000	0.0000	0.0000	+H	[M+H]+
76.0660	50.0000	0.0000	0.0000	-CH3	NA



PeakForest project



contact@peakforest.org

