

➤ PeakForest HOWTO

Add a compound

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➤ Introduction – PeakForest

Access

The screenshot shows the website nightly.peakforest.org in a browser. The page features the PeakForest logo (an owl and a mountain) and the text "the MetaboHUB's Spectral Database, a nightly version (dev)". Below the header, there are five blue buttons arranged in two rows: "PeakForest - WebApp" (top left, highlighted with a red box), "REST webservice (v2)" (top middle), "Documentation (v2)" (top right), "REST webservice (v1)" (bottom left), and "Documentation (v1)" (bottom middle). Red arrows point from three text boxes to these buttons: "WebApp: web application for users" points to the "PeakForest - WebApp" button; "API REST API: for programatic access" points to the "REST webservice (v1)" button; and "REST API: technical doc" points to the "Documentation (v1)" button. The browser's address bar shows the URL <https://nightly.peakforest.org/webapp/>.

WebApp: web application for users

PeakForest - WebApp

REST webservice (v2)

Documentation (v2)

REST webservice (v1)

Documentation (v1)

API REST API:
for programatic access

REST API:
technical doc

➤ Introduction – PeakForest

Menus and Authentication

The image displays two screenshots of the PeakForest web application interface, illustrating the navigation and authentication process.

Top Screenshot (Main Interface):

- The browser address bar shows `nightly.peakforest.org/webapp/`.
- The sidebar menu (highlighted with a red box and labeled "Menus") includes:
 - Search
 - Peak Matching
 - Stats and API
 - Tools
- The main content area features the PeakForest logo (an owl) and the text "a spectral data portal for Metabolomics community".
- The top right corner contains a "Login or Register" button (highlighted with a red box and labeled "Authentication") and a "Log in / register" button.

Bottom Screenshot (Login / Register Modal):

- The modal form is titled "Login / Register".
- It includes tabs for "Login" and "Register".
- The "Login" tab is active, showing input fields for email/username and password (highlighted with a red box and labeled "Authentication form").
- Buttons for "Close" and "Login" are present at the bottom.

➤ Introduction – PeakForest

The screenshot shows the PeakForest Nightly web application interface. The browser address bar displays `nightly.peakforest.org/webapp/home`. The left sidebar contains a menu with the following items: Search, Peak Matching, Add ..., Stats and AP, Tools, Curation, and Backoffice. The main content area features the PeakForest logo (an owl) and the text "a spectral data portal for Metabolomics community". Below this is a search input field with the placeholder text "e.g. Glucose" and an "Advanced" button. The bottom of the page includes links for "Contact", "About", "My PeakForest", and "metaboHUB".

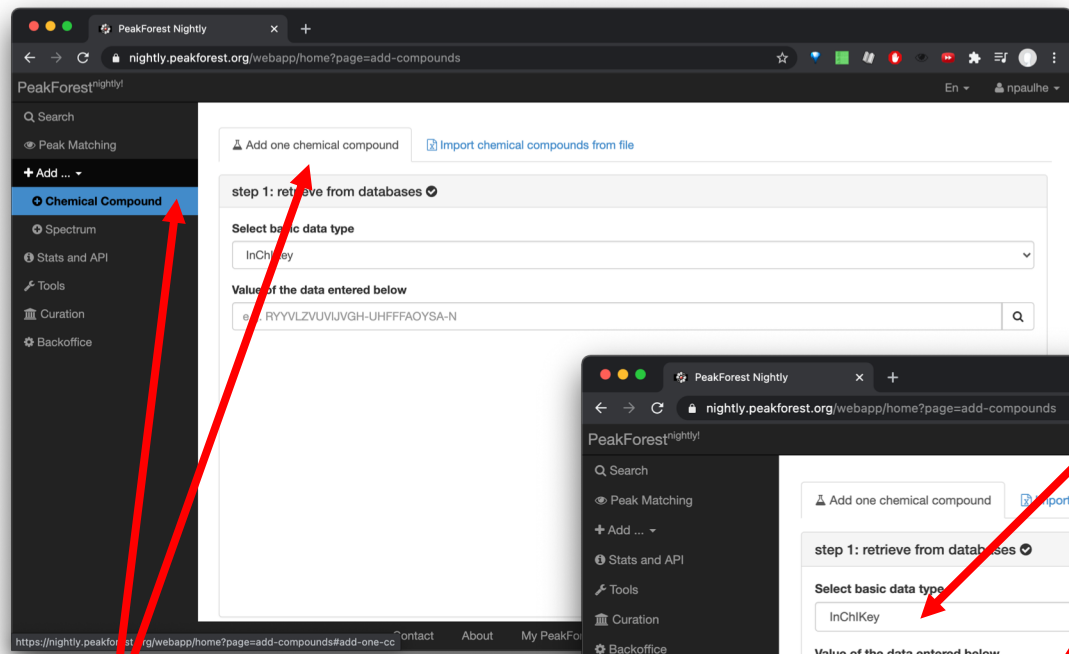
Four callout boxes describe user roles and their associated options:

- Options « user »** (red box):
 - Login update
 - Token
- Options « anonymous user »** (red box):
 - Searches, matching
 - Informations and indicators
- Options « validated user »** (orange box):
 - Add compounds
 - Add spectra
- Options « curator user »** (purple box):
 - Read, manage curation issues
- Options « administrator user »** (blue box):
 - Users management
 - Database supervision

Arrows indicate the mapping of roles to interface elements: the "user" role is linked to the user profile dropdown; the "anonymous user" role is linked to the Search and Peak Matching menu items; the "validated user" role is linked to the Add ... menu item; the "curator user" role is linked to the Curation menu item; and the "administrator user" role is linked to the Backoffice menu item.

➤ Add one compound

1/3 – Search if any entry does not already

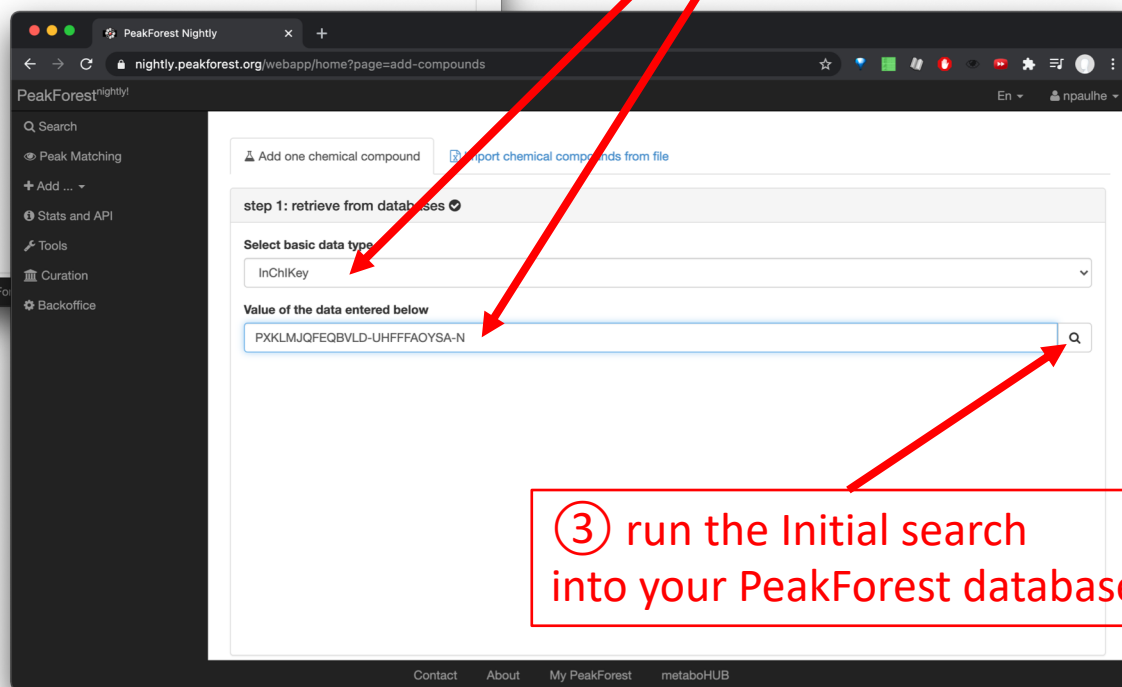


① Add menu

- Chemical compound
- Add ONE chemical compound

② Initial search

- By common name
- Or by InChIKey



③ run the Initial search into your PeakForest database

➤ Add one compound

2/3 – Checkings OR new online search

PeakForest Nightly

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

PeakForest^{nightly}

Q Search

Peak Matching

+ Add ...

Stats and API

Tools

Curation

Backoffice


En npaulhe

1 If the compound already exists

- Properties checkings

step 1: retrieve from databases

step 2: select compound to add

Chemical Name	Monoisotopic Mass	Formula	Structure
Bis(4-hydroxyphenyl)methane	200.0837296	C ₁₃ H ₁₂ O ₂	

If your compound is not listed above, run a Deep search Q

2 If not, deep search using the « CTS » service

3 Select the right compound into query results

PeakForest Nightly

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

PeakForest^{nightly}

Q Search

Peak Matching

+ Add ...

Stats and API

Tools


Curation

Backoffice

En npaulhe

step 1: retrieve from databases

step 2: select compound to add

Chemical Name	Monoisotopic Mass	Formula	Structure
Bis(4-hydroxyphenyl)methane	200.0837296	C ₁₃ H ₁₂ O ₂	

If your compound is not listed above, run a Deep search Q

Chemical Names	Monoisotopic Mass	Average Mass	Formula
4,4'-Dihydroxydiphenylmethane,4,4-Methylenediphenol,4-[[4-hydroxyphenyl)methyl]phenol,Bis(4-hydroxyphenyl)methane,4-(4-hydroxybenzyl)phenol,4-(4-Hydroxybenzyl)Phenol,Bisphenol F	200.0837296	200.23318	C ₁₃ H ₁₂ O ₂

Contact About My PeakForest metaboHUB

➤ Add one compound

3/3 – Data validation

① Mandatory

- structure
- names (scores)
- Cross-ref bank ids

② (optionnal)

- Curation message(s)
- Bibliography reference(s)

③ Validation

PeakForest Nightly

nightly.peakforest.org/...

PeakForest^{nightly}

Q Search

Peak Matching

+ Add ...

Stats and API

Tools

Curation

Backoffice

Add one chemical compound

Import chemical compounds from file

step 1: retrieve from databases

step 2: select compound to add

step 3: validate / add data

☐ 2D ☒ 3D

Name Bisphenol F

Formula C₁₅H₁₂O₂

Monoisotopic Mass 200.0837296

Average Mass 200.23318

Download [Mol](#)

Smile Oc1ccc(cc1)Cc1ccc(cc1)O

InChI InChI=1S/C13H12O2/c14-12-5-1-10(2-6-12)/9-11-3-7-13(15)8-4-11/h1-8,14-15H,9H2

InChIKey PXKLMJQFEQBVL-DUHFFFAOYSA-N

Names

Bisphenol F	★★★★★ 5.0
Bis(4-hydroxyphenyl)methane	★☆☆☆☆ 1.0
4,4'-Methylenediphenol	★☆☆☆☆ 1.0
4,4'-Dihydroxydiphenylmethane	★☆☆☆☆ 1.0
p-hydroxydiphenylmethane	★☆☆☆☆ 1.0
bisphenol F	★☆☆☆☆ 1.0

☒ new name

PubChem CID 12111

ChEBI CHEBI:34575

KEGG C14298

No accepted citation.

[Add bibliography ref.](#) [Add curation message](#) [Validate](#)

Contact About My PeakForest metaboHUB

PeakForest project



contact@peakforest.org

