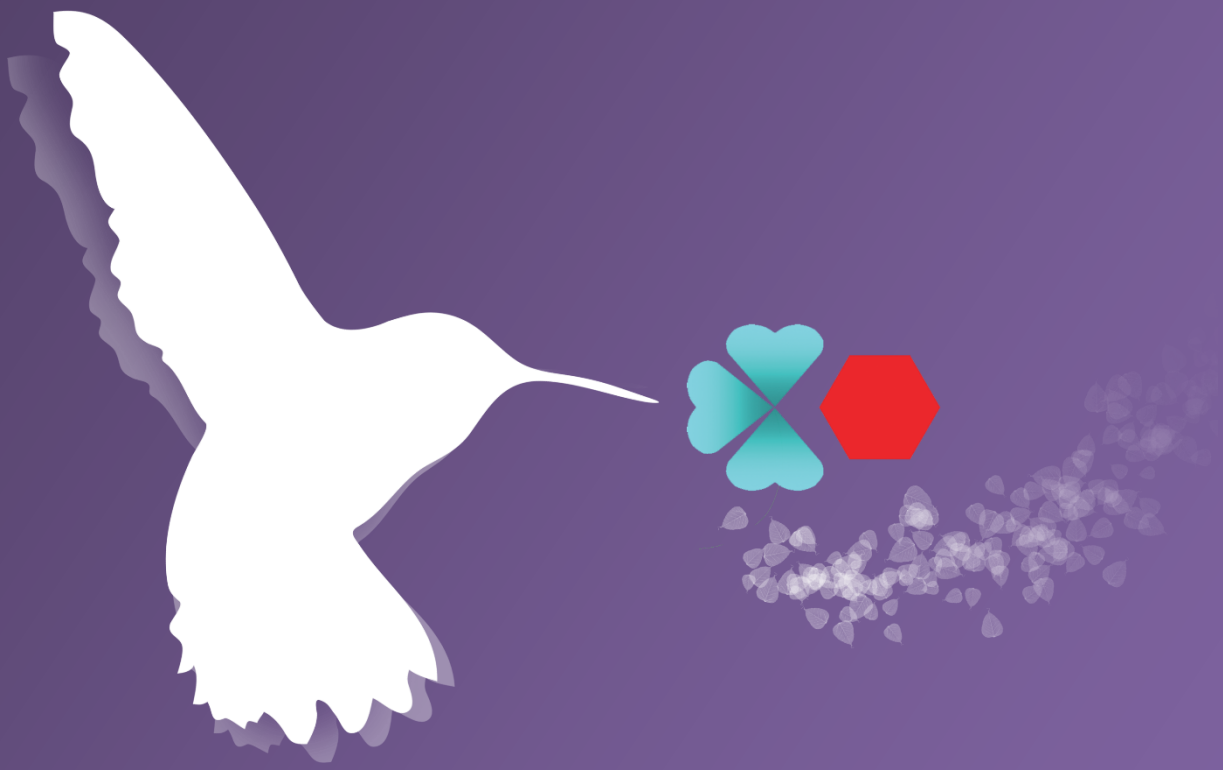
2024

L-g-Chimio V1.7



ChemBioFrance

cnrs

Contents

I. User Manual

A. Connection

1. Login to the application

A user's connection to the application is done through the left menu *(see red box* Image 1) by entering your **username** and **password** automatically sent by email when the user is created by the administrator/chemical librarian. Then, click Connection. If you are correctly authenticated, you arrive on the home page of your laboratory's chemical library (Image 2). Otherwise, you return to authentication, with the possibility of requesting a password again (Image 3) by clicking on the link “Lost password” see chapter: I.A.2.

Image 1: Login to the application

Image 2: Chemical librarian/administrator user authentication successful

Image 3: Error during user authentication

2. Forgot your password

If you have lost your password, you can obtain a new one automatically. At the bottom of the login menu, you click on the link “Forgot your password? » you arrive on a page (Image 4) where you simply enter your name (pay attention to upper and lower case letters) as well as your email address and submit to receive a new password. **Please note, the email address provided must correspond to the one known for the corresponding account.**

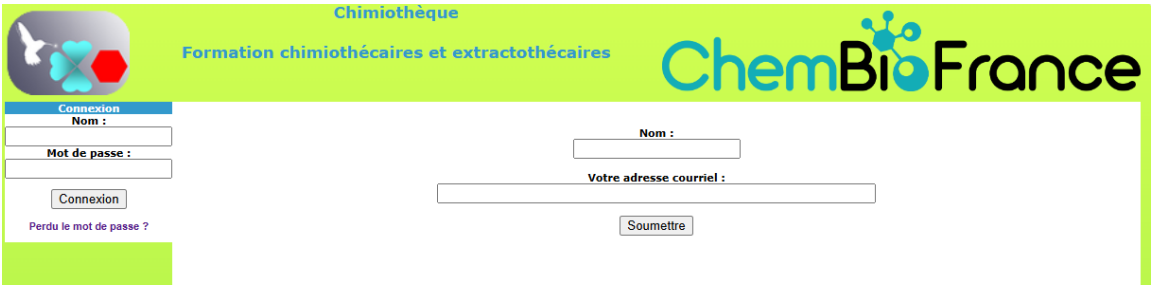


Image 4: Page to obtain a new password automatically

B. Chemical Library Part

1. Entering a new product

a) First entry page

In the entry section of the Chemical Library Menu, you arrive at the entry of a new product (Image 5), this section is accessible to all. There is a difference for the administrator and the manager who will have to enter the name of the chemist, to do this type the 1st letter of the name and select it from the drop-down menu. As a reminder, the chemist account must first have been created. All fields marked with a * must be completed in order to continue.

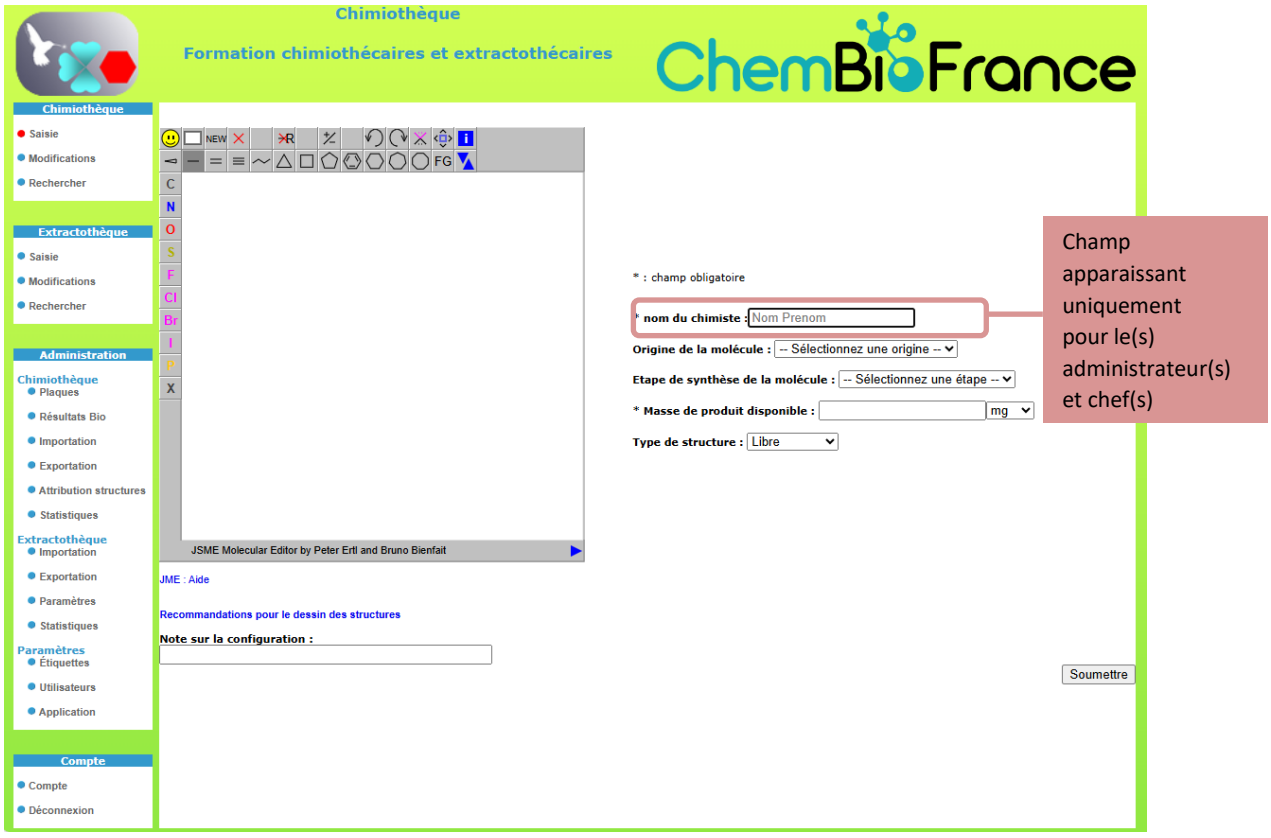


Image 5: Entering a new molecule

Below this, you have a link to a PDF file containing the recommendations of the National Chemical Library, particularly those concerning the drawing of molecular structures. You can also find this document in the Appendix to chapter 1.a.i.1.A

You can directly import your molecular structure into JSME ©*Novartis Institutes for BioMedical Research Inc. and Bruno Bienfait* from a mol file or a smile. For example from the Biovia Draw © Dassault Systemes software, once your molecule has been drawn or opened in the software, click on the "Edit" menu then on "Copy As" then click on "Molfile" or "Smiles" (Image 6). If you have sugars, choose the Smiles code, because upon import you will have a molecule automatically redrawn closer to the standard that we recommend.

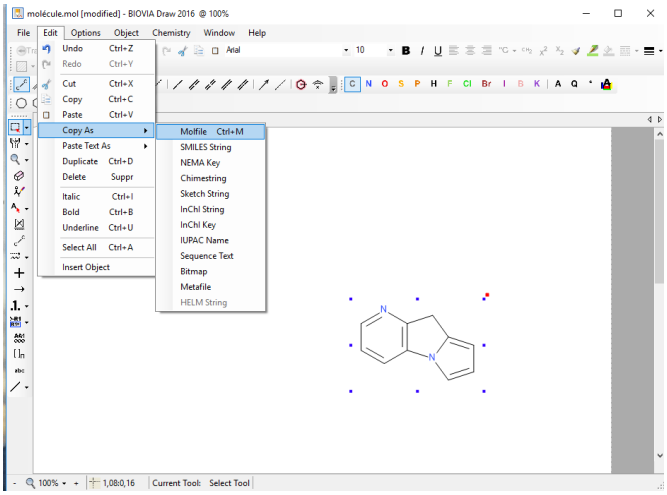


Image 6: copy your structure in Mol format from structural drawing software

In Lg-Chemio you click on the icon  (or right click in the window) then click on “Paste MOL or SDF or SMILES” in this new window paste (Crtl V) your text (Mol or Smiles) from your software structure drawing then click on the “Accept” button (Image 7).

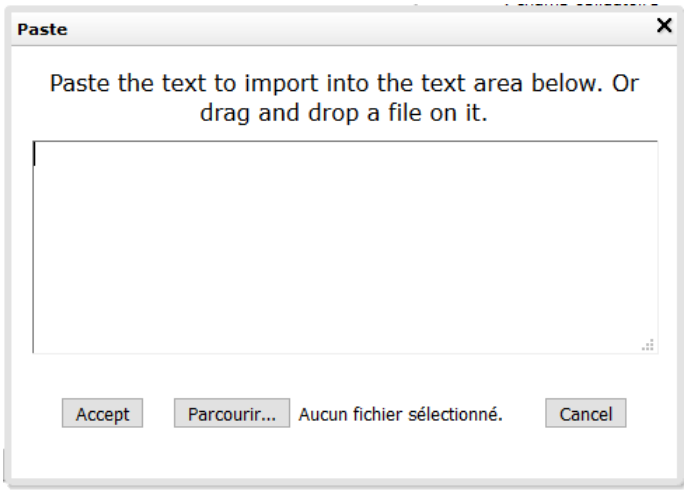


Image 7: JSME window or paste your text in Mol or Smiles format

The “Note on configuration” field allows you to write a detail not visible on the structure drawing, for example: mixture of enantiomers.

Attention, il est très important de prendre soin de bien dessiner votre structure moléculaire, car c’est l’élément central du système.

Once the molecule has been correctly drawn, you must enter the mass in mg or nmol of product placed in a pill bottle. The nmol unit is used for the European Glycomimetics Chemical Library.

It can be 0mg. The product is entered for memorandum (*the product remains laboratory know-how)* , it is therefore available to be screened virtually.

Then, you must enter the type of the molecule to know if it is:

- **Royalty free** : the molecule is visible to everyone. The molecule can be exported to the National Chemical Library.
- **Under contract** : the molecule is visible to the user who entered it, to their manager, to their boss and to the administrator.
- **Patented** : the molecule is visible to everyone. You will have an additional field allowing you to enter the patent number on the second page.

The “origin of the molecule” field contains a default value for all users, if it has been defined in the “Parameters” section (see Chapter **Erreur ! Source du renvoi introuvable.**), you must select another value if the default one is not suitable for your laboratory.

Once the fields are completed correctly, click on the “Submit” button to proceed to the next page. Example of entry, see Image 8.

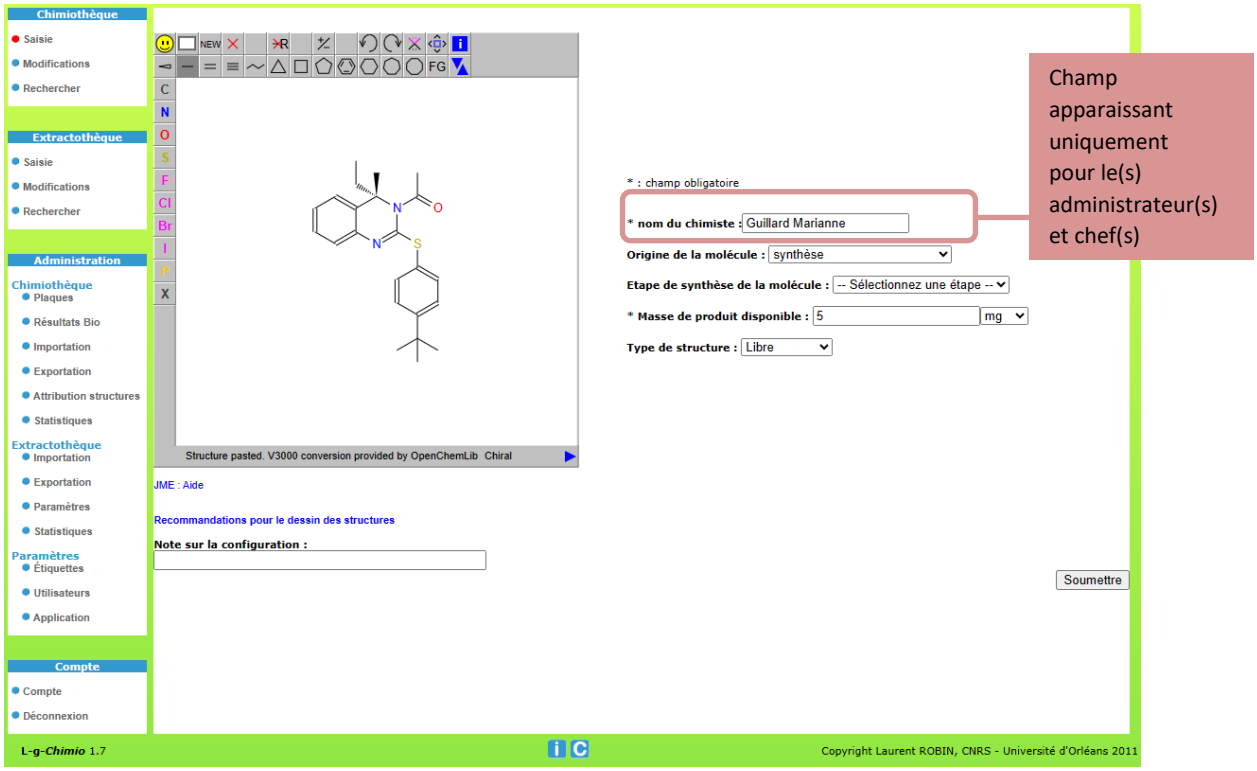


Image 8: Example of entry with an administrator view

If the structure is already present in the database, the message “ *Attention duplicate!” the structure already exists in the database. Do you want to continue ?* » is displayed, you can choose to accept this duplicate or cancel the entry see Image 9.

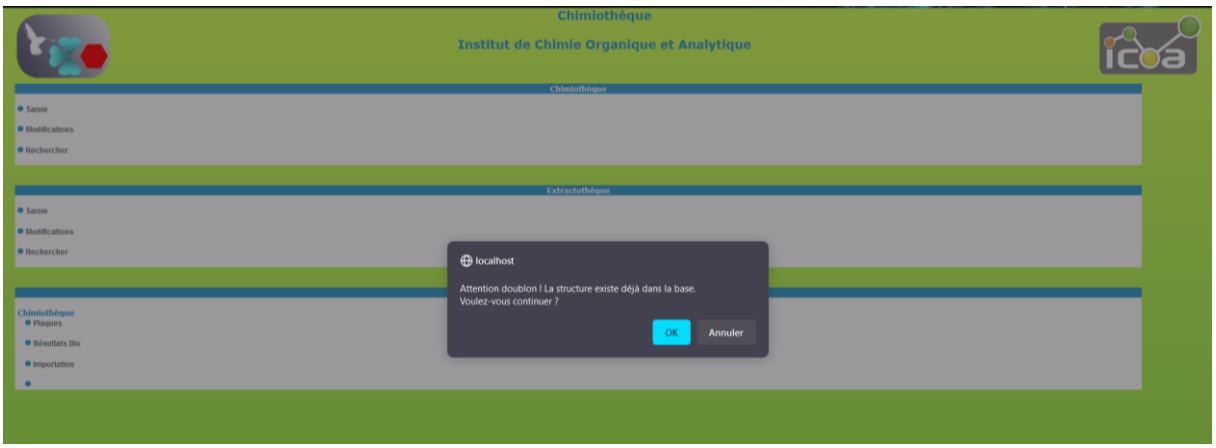


Image 9: Example message for a duplicate structure

b) Second entry page

If you have set the numbering to automatic (Chapter **Erreur ! Source du renvoi introuvable.**), the number appears in red at the top in the middle. You will find an example of the second entry page in the chemical library in Figure 10. Otherwise you will have to manually enter your product number in the corresponding field.

At this point you can still change the mass. If it is below the threshold adopted in the configuration section (Chapter **Erreur ! Source du renvoi introuvable.**), (*in our example 5mg*), the number is modified automatically if you are in automatic numbering when your cursor changes field. In this example, we chose to enter the mass at 5 mg on the first page. I get the number ICOA-FST-L-01A02. If we increase this mass on page No. 2, the number is not modified. On the other hand, if we decrease below the 5 mg threshold defined in the settings (Chapter **Erreur ! Source du renvoi introuvable.**), the number is automatically modified and becomes ICOA-FST-L-1, representing a product number not stored. **A number proposed on page No. 2 of the entry is reserved for the day, even if the user does not complete his entry or if he modifies the mass resulting in a change of number. This number will be offered again from the next day.**

Likewise, if a product is out of stock (0mg), this results in an automatic number change when the user makes the mass change. The number thus released will be automatically offered at the next entry made by a user. For each entry in the app, there is **a random permanent unique 8-digit number** that is generated. This number visible in the product sheet can be used for data transfer and dialogue with the National Chemical Library or biologists. Thus each product has a unique random and permanent 8-digit number and a storage number according to the settings defined in the **Erreur ! Source du renvoi introuvable.**.

For analyses, you can enter the analysis results in text form in the white box and/or enter the spectrum file via the “Browse” button. There is no lock on file type. However, we recommend that you use a long-lasting format such as “PDF” and not too large, because it is stored in the database.

Trick :

In the “Precaution” field, selecting or deselecting an entry can be done using the Alt Gr key on your keyboard + left mouse click.

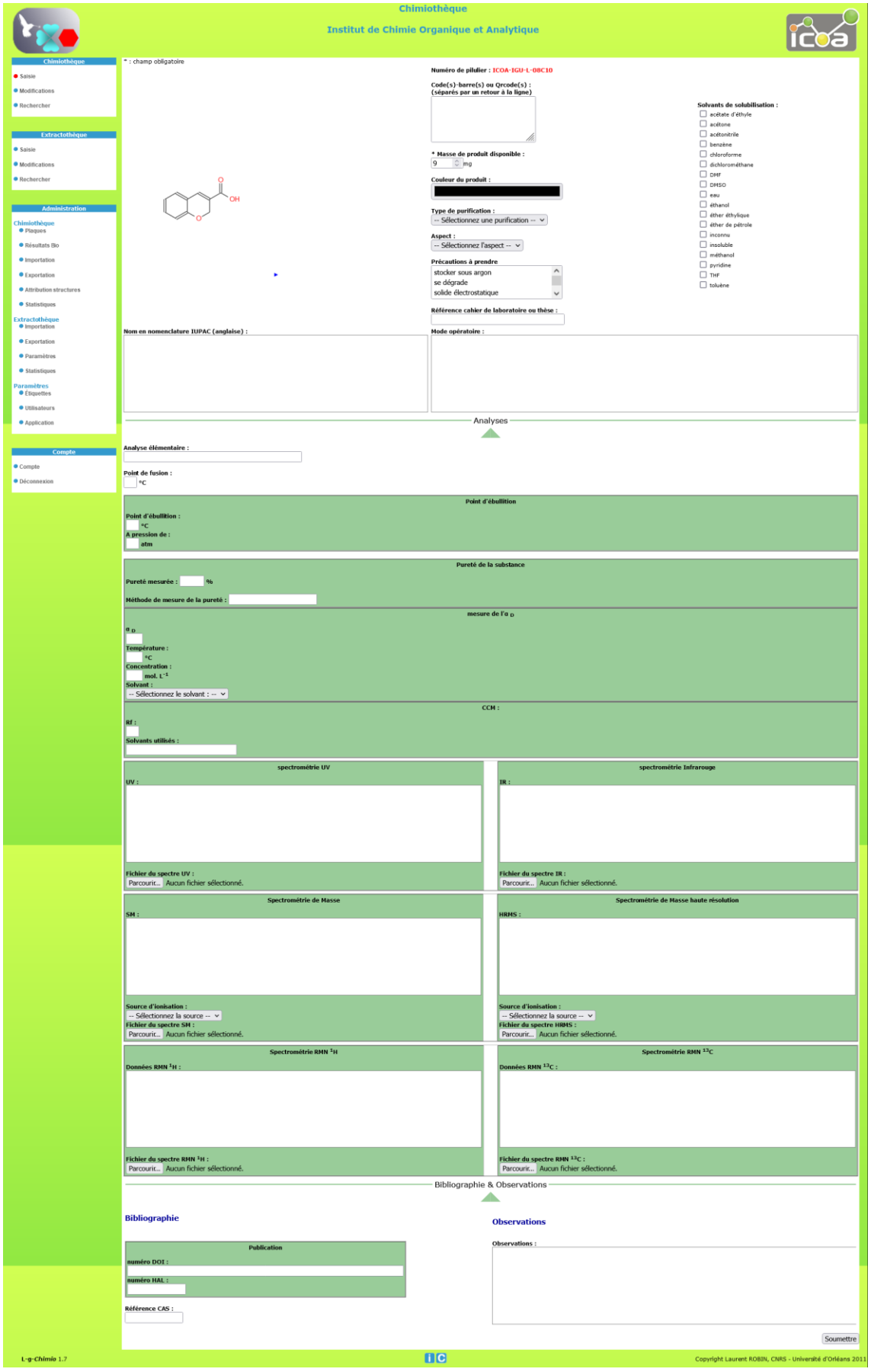


Figure 10: Example of entry

All information provided, click “Submit”. **At that time, only the information is saved in the database.** An automatic email is sent to the manager, boss and administrator. An option in the “Account” section allows everyone to deactivate this return by email, see the I.D.

2. product data

The “Modification” section of the left “Menu” allows the user to consult and modify their molecules, for managers or leaders, those of their team. The administrator can intervene on all files.

a) Perform a search

The home page of this section allows the user to search according to various criteria.

Everyone can search by exact structure, by substructure, by similarity, by molar mass, raw formula, laboratory notebook/thesis reference, tags and numbering. For the latter, you can use:

- either the unique random 8-digit number,
- either the number defined in the “product-parameters” section (example: ICOA-FST-L-01A02 see Chapter **Erreur ! Source du renvoi introuvable.**),
- or the number of the National Chemical Library (CN000000V) if it was imported by the administrator (Chapter **Erreur ! Source du renvoi introuvable.**).

Regarding the molar mass and the crude formula, you can perform an exact search by checking the “exact” box. Otherwise, by default you search by pattern.

For searching by tags you can select one or more tags (Ctrl key + left mouse click).

The upper part of the page is modified depending on the user (*chemist, manager, chef and administrator (* Image 12*)*

The chemist (Image 12) will see the “molecule type” field *(free, under contract or patented)* , the manager (Image 13) will see the “molecule type” and “collaborators” field *(with only the members of his team),* the leader (Image 14) will see “teams” *(with his or her teams attached)* .

The administrator will have all the menus with all the teams and users (Image 11).

To search by exact structure, substructure or similarity you must draw your structure in JSME © *Novartis Institutes for BioMedical Research Inc. and Bruno Bienfait* then click on the desired search type. For similarity search you can adjust the Tanimoto coefficient using the tab. The closer it is to zero, the less restrictive your search will be .

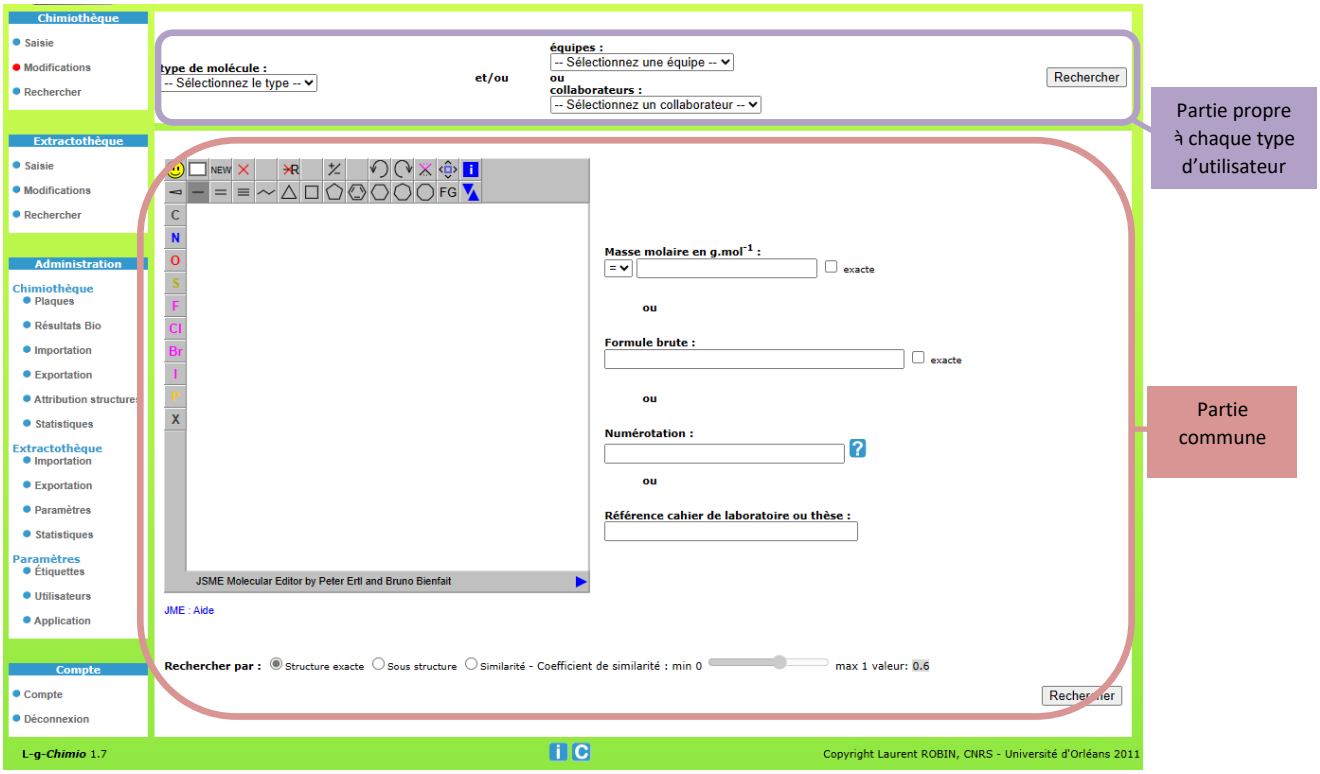


Image 11: search page seen by the administrator

Image 12: Display seen by the chemist guy

Image 13: Display seen by the responsible guy

Image 14: Display seen by the boss guy

Thanks to this form, the user can access for research, modification and consultation only the products that are attached to him by the hierarchy of rights (Erreur ! Source du renvoi introuvable.**). Only the administrator will have a view of all the teams defined in the** Erreur ! Source du renvoi introuvable..

b) Result of the research

After entering a search criterion and clicking on “Search” in the relevant section, you obtain a result which is displayed page by page with 8 molecules per page (Image 15).

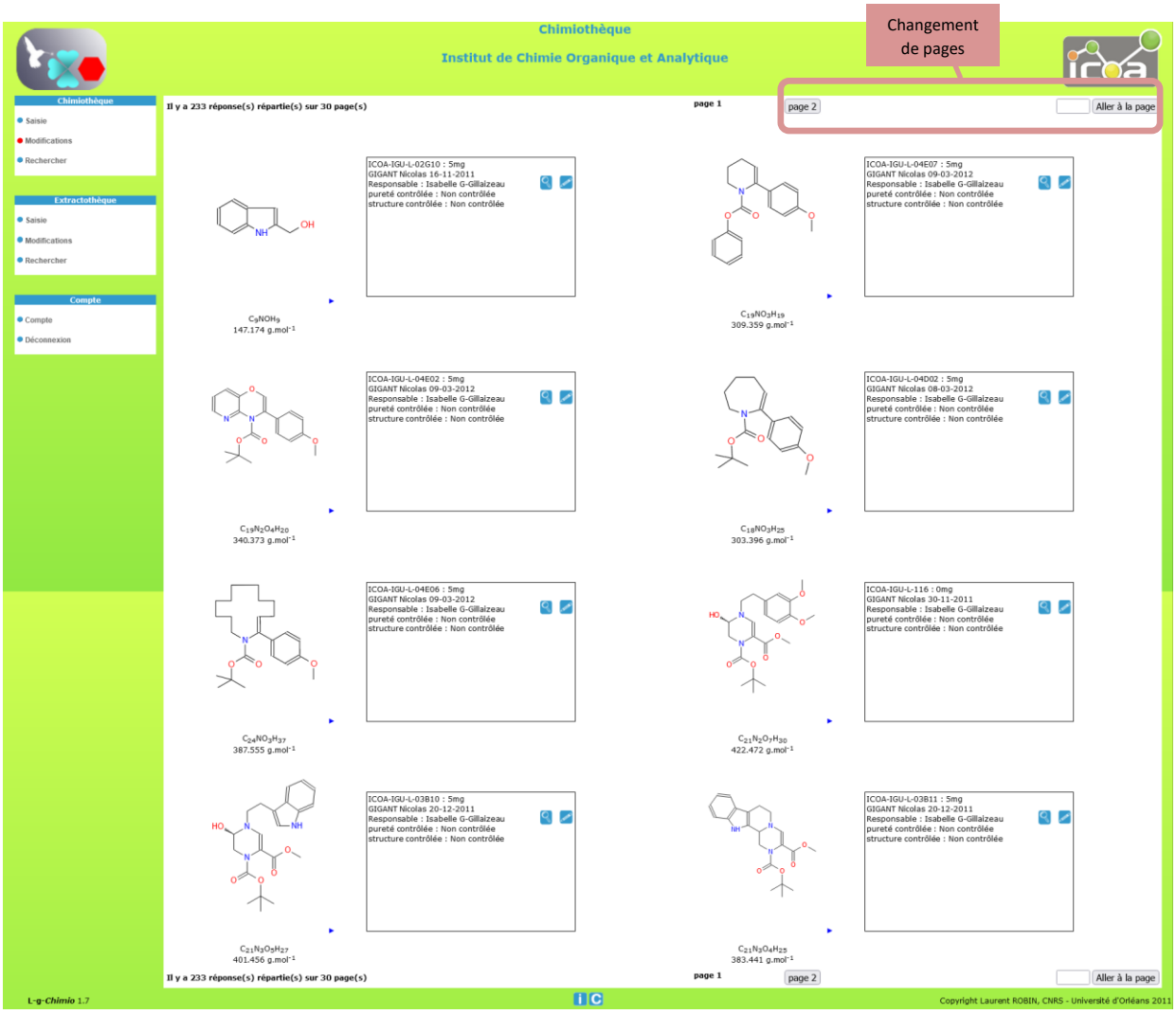


Image 15: Results of a chemist view search

At the top and bottom of the results page, you can change pages, either page by page, or you can go directly to a specific page. The results page displays the structure with the raw formula and the corresponding molar mass. In front of the structure, you have the reference of the file(s) with the storage number, the mass stored, the name of the user who filled in the file and the date of entry, but also the name of the person responsible and the information on purity and structure control. **Since duplicates are accepted by the system, you can have several records for the same structure** (Image 16)

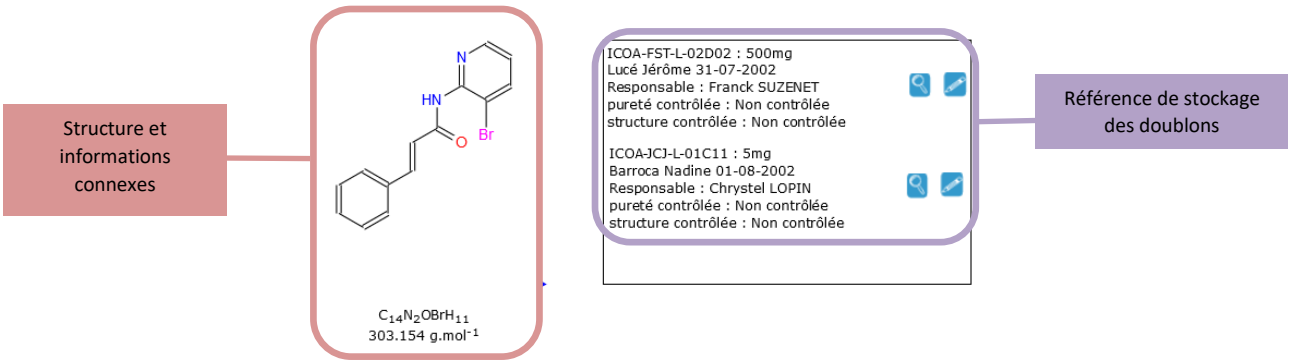


Image 16: Existence of two files for the same structure

If you wish to consult your file, click on the icon: , if you wish to modify the data of one of your files, click on the icon: .

Trick :

You can copy (in text format) a structure that interests you directly from the result page. Right-click on the structure, you obtain a menu (Image 17).

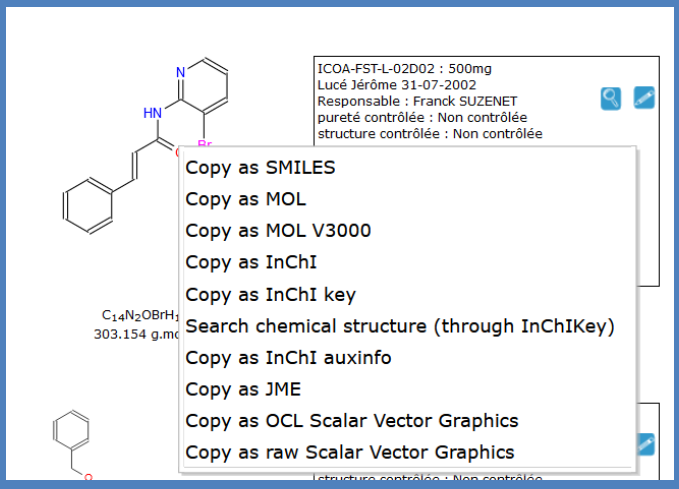


Image 17*: JSME menu*

This allows you to copy the molecular structure in mol type text format (other formats are available: Smiles, InChI). Then copy the text into a text editor (notepad, wordpad, etc.) and save to a file with the “mol” extension.

c) Consult a file

If you clicked on the icon in the search results page, you access the consultation of the substance sheet. This is modulated according to the user's rights.

Image 18*: Menu of the consultation form*

All users have the “Structure” and “Analysis” tabs. The manager and administrator also have the “Organic Results” tab. However, only the administrator has the “History” tab.

(1) “Structure” tab

For the first tab (

Image 18), you visualize all the data of the structure. They are divided into four categories: data entered by the user, data calculated by the system and data imported by the administrator.

- The data entered by the user which are displayed on this tab are the 2D structure, the operating mode, the observations, the color of the substance, the mass of the product stored in mg, the origin of the molecule, the type of product, the experimental elemental analysis, the type of purification, the laboratory notebook reference, the melting point, the boiling point, the special precautions to be taken with regard to the product, the solubilization solvents of the substance, bibliographic references:
  - the DOI number (https://fr.wikipedia.org/wiki/Digital_Object_Identifier),
  - the CAS number (https://fr.wikipedia.org/wiki/Num%C3%A9ro_CAS),
  - the HAL number (https://fr.wikipedia.org/wiki/HAL_(archive_ouverte))
- The data calculated by the system are theoretical elemental analysis, molar mass and crude formula.
- The data generated by the system which is visualized on the form are the storage number, the constant number, the date of entry, the name of the person who entered the data.
- The data imported by the administrator are the number of the National Chemical Library and the tare of the pillbox see chapter: **Erreur ! Source du renvoi introuvable.**.
- For Chemistry Libraries that have used previous versions of Lg-Chimio you have data at the field level: Logp, check Lipinski's rules, Number of acceptors, Number of rotary links, Number of aromatic atoms, Number of aromatic bonds, Number of donors, Number of asymmetric atoms, Fusion point, Boiling point. These data were calculated by the Chemaxon company tools which we no longer use in this new version.

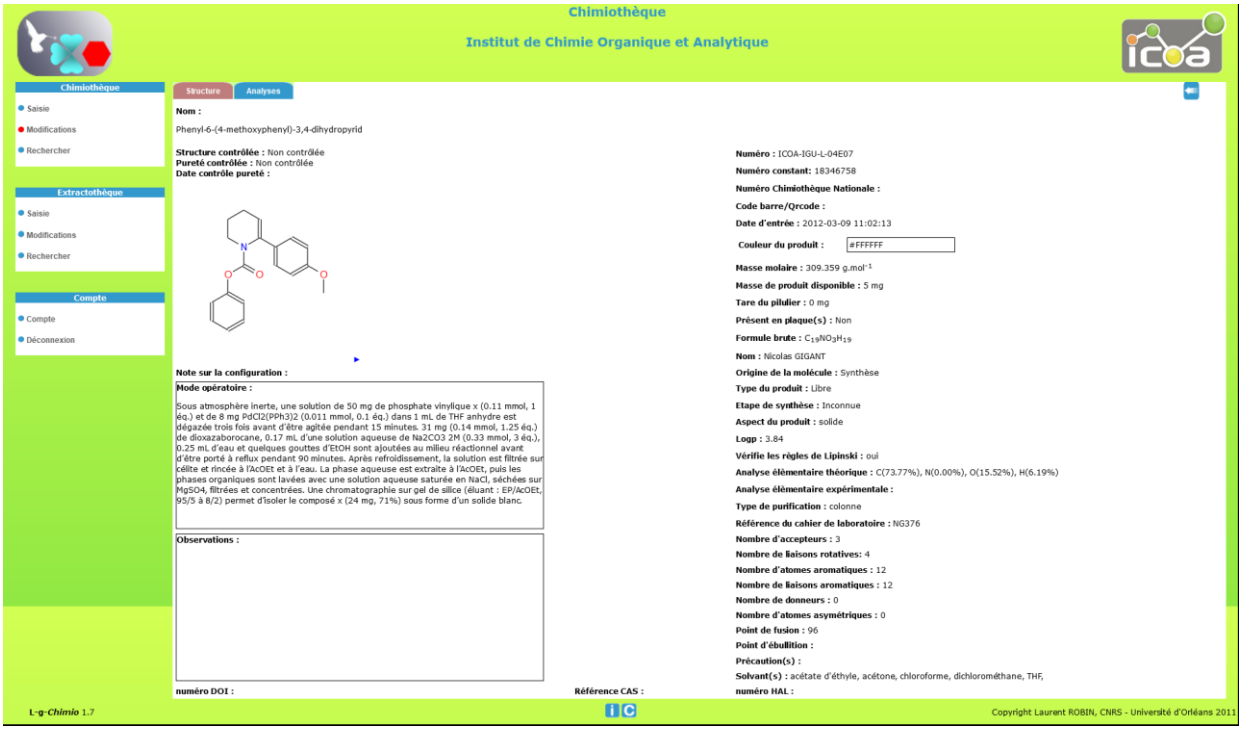


Image 19: "Structure" tab

(2) "Analysis" tab

In the "Analysis" tab (Image 20), you can view all the results of the analyzes carried out on the substance, which have been entered by the user. On the left side you have the numerical results and on the right side you have the files uploaded by the user and available for download.

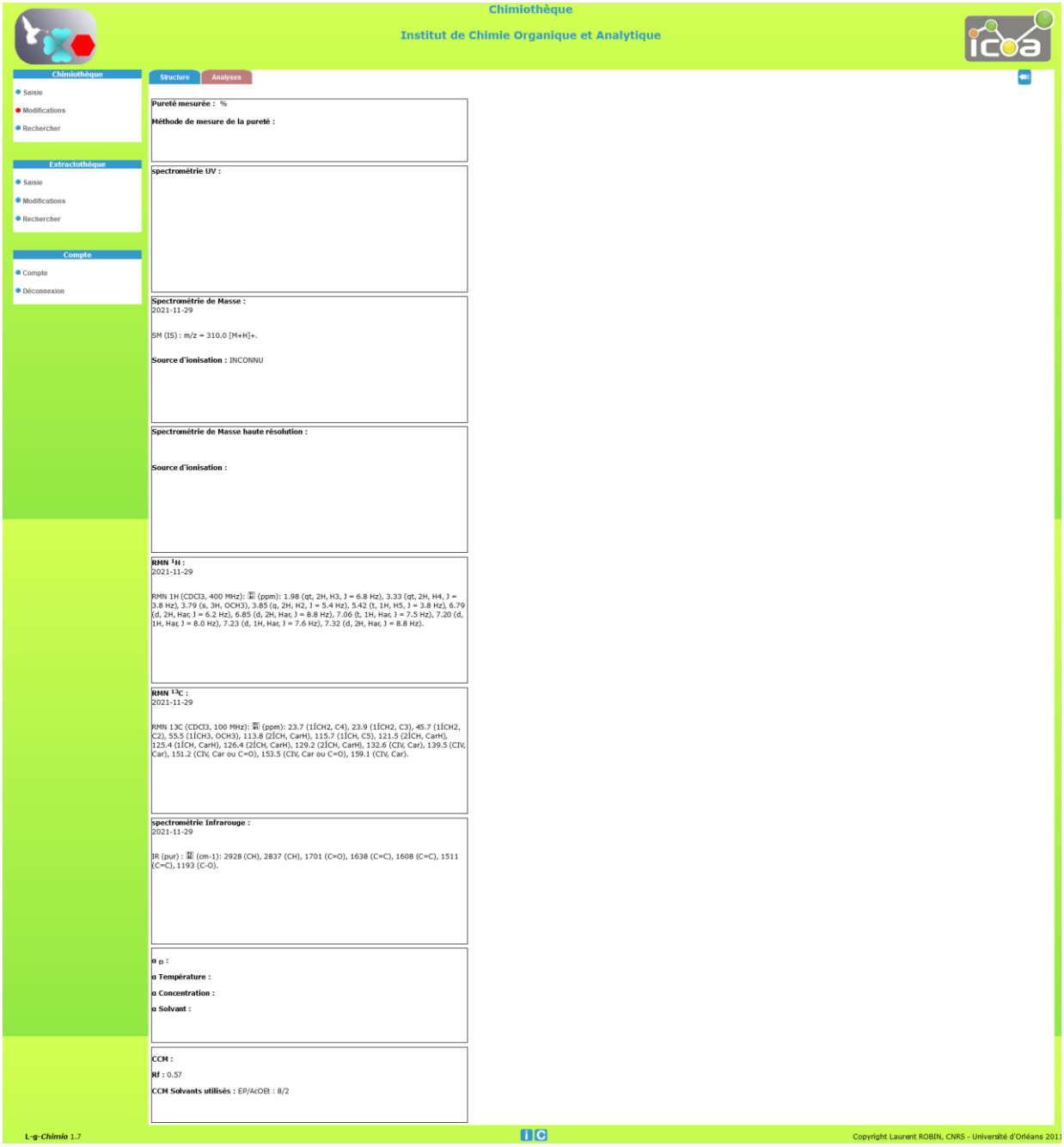


Image 20: "Analysis" tab

(3) "Organic Results" tab

The "Organic Results" tab, accessible only to managers, bosses and administrators, allows you to have in tabular form the results of all the biological tests carried out on the substance consulted (Image 21). A result only appears if it was imported by the administrator using the import tools (see: Chapter **Erreur ! Source du renvoi introuvable.**).

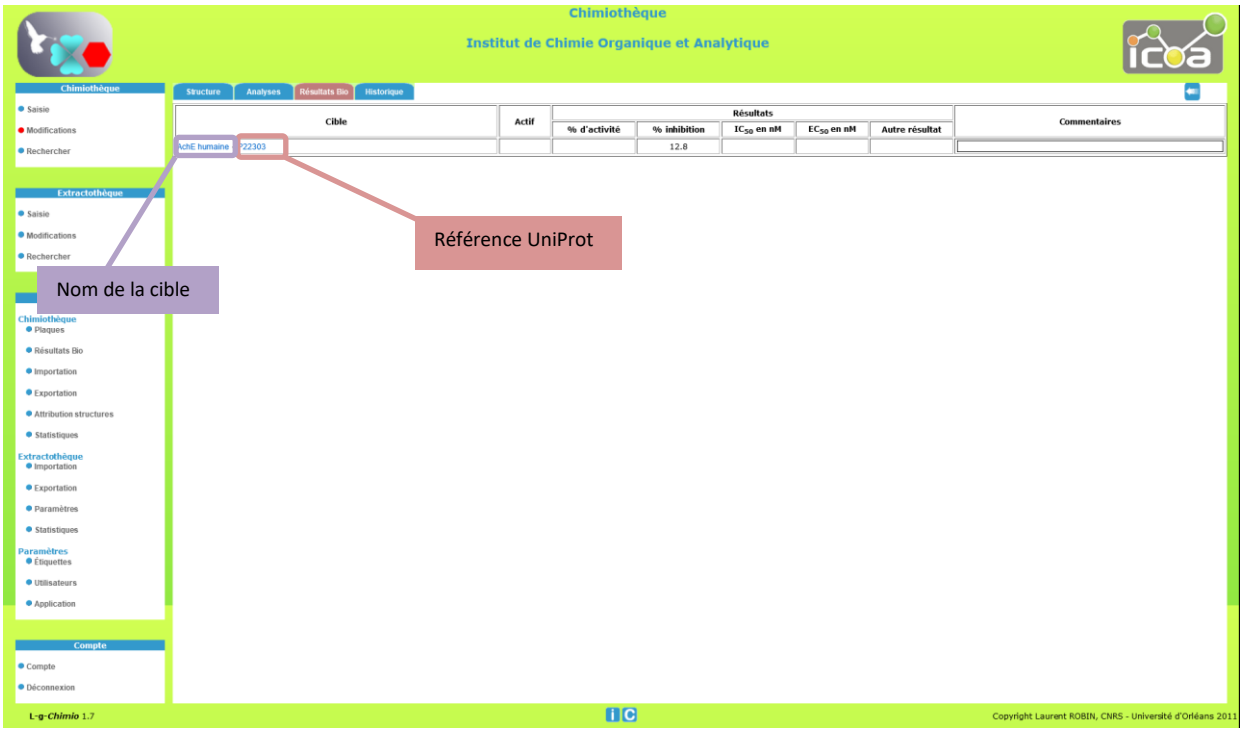


Image 21: "Organic results" tab

By hovering over the name of the biological test, you access the details (Image 22). The number next to the name of the biological test here P22303 on Image Image 22it is the UniProt reference (https://fr.wikipedia.org/wiki/UniProt) of the protein, by clicking on it, you are directly taken on the data for this protein on the UniProt website.

Image 22: display of biological test details

(4) "History" tab

This tab is only accessible to administrators (Image 23). It allows you to view the history of changes made on the substance sheet consulted. This historization provides the following information in table form: the field that was modified, by which person, on what date, we also have the old value of the field.

Image 23: example of a file modification history

(5) Export a search

In administrator mode, you can export your search using the export button at the top right of the page see Image 24.

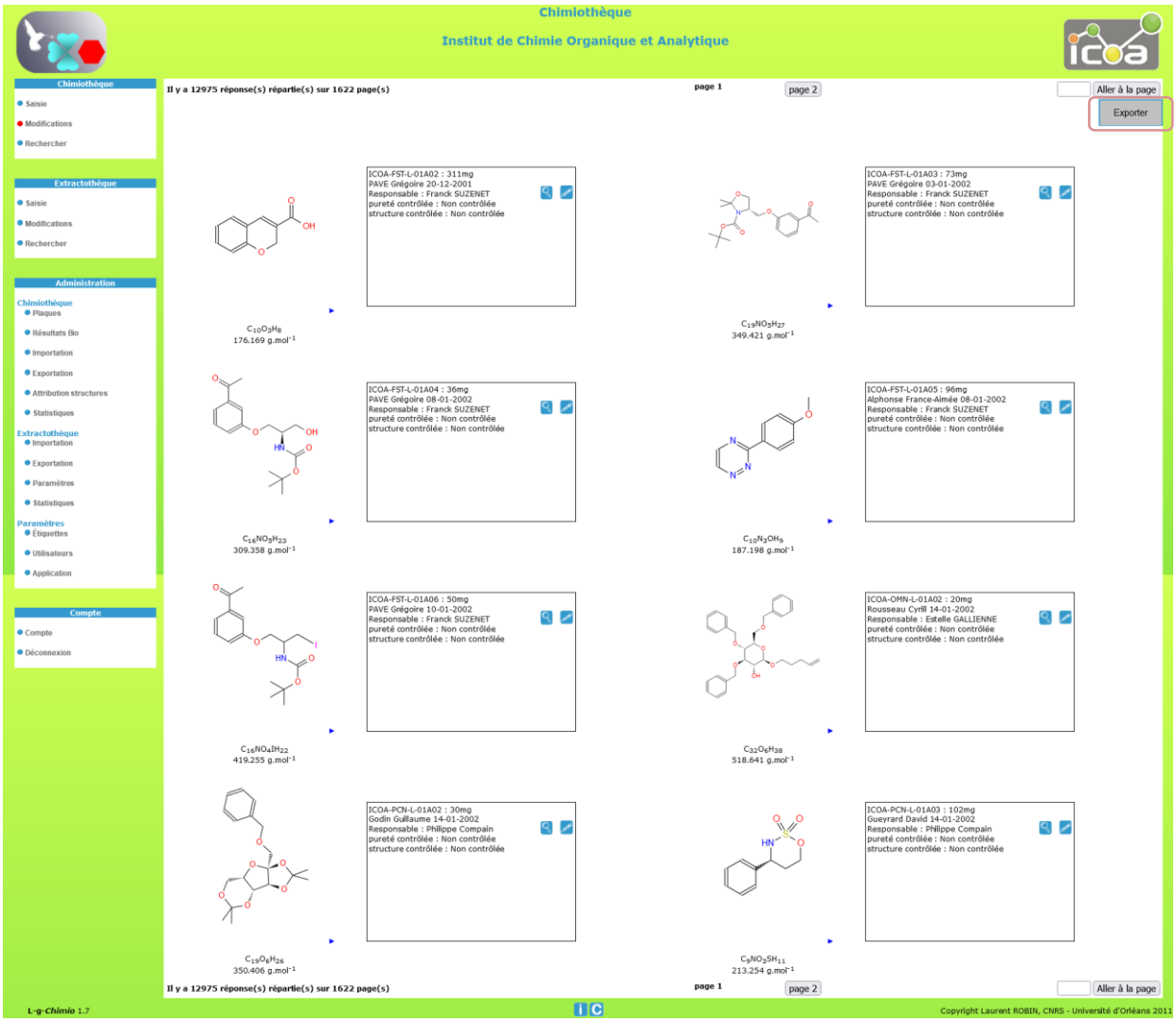


Image 24: exporting a search from the "modifications" tab

By clicking on this export button, two choices will be displayed on your screen, see Image 25:

- either you can copy all the storage numbers to the clipboard,
- or you only export the 8 storage numbers of the displayed page.

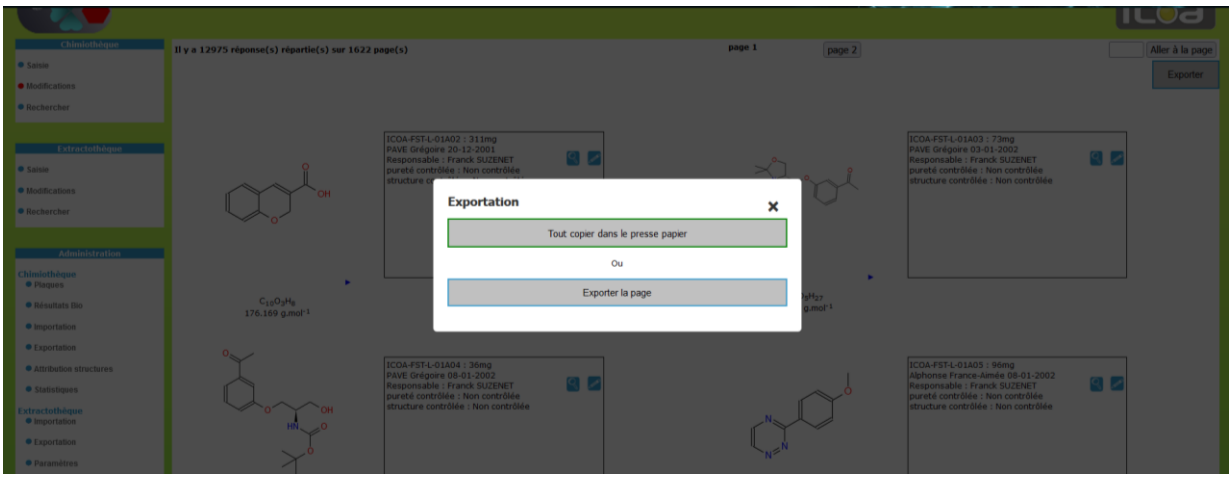


Image 25: Choice between the 2 export options

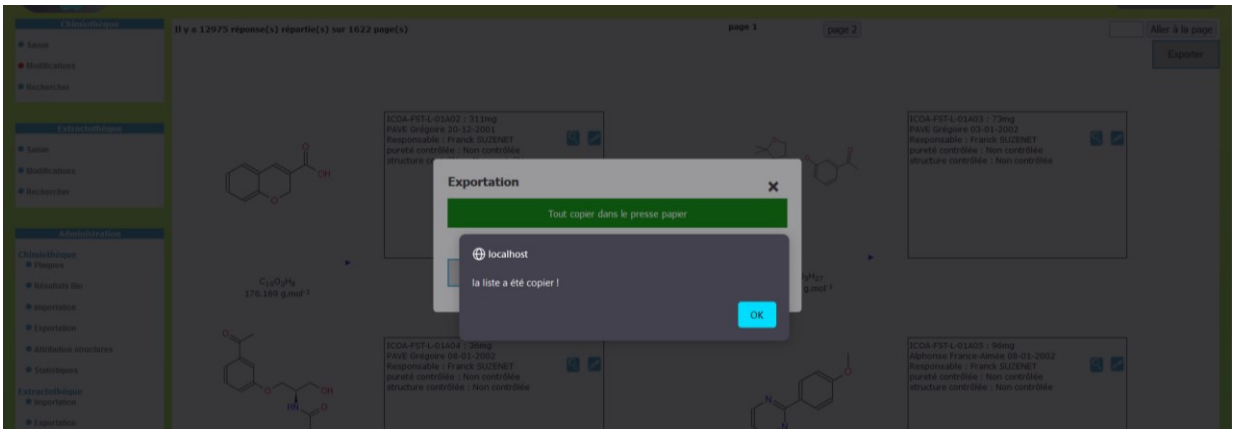


Image 26: Copying the list to the clipboard

Image 27: exporting the list of the visible page (8 results) in the export page

Once copied, you can paste the whole thing, for example, into the export tab of the chemical library part of Lg-chemo. This will allow you to extract the data in SDF form see chapter **Erreur ! Source du renvoi introuvable.**.

d) Edit a record

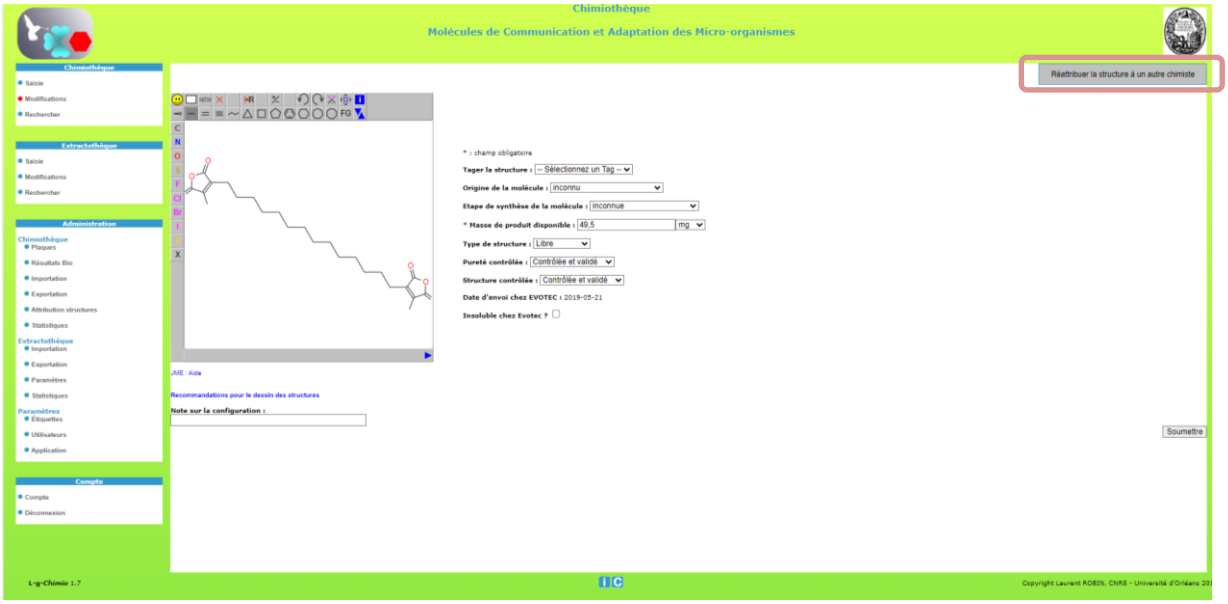
From the page of your search results , if you clicked on the icon, you arrive at the modification of the substance sheet. This is modulated according to the rights of the connected user. The form on which you arrive is identical to that of the entry (chapter I.B). For all users except the administrator, the “structure type” field is disabled. Only the administrator can modify the type of structure *(Free, Under contract or patented*), because this change of state implies, if you are in automatic numbering, a modification of the physical storage number.

If you are on automatic dialing and the mass of the product is changed, within 7 days of the initial entry of the substance. So, a modification of the storage number (chapter Erreur ! Source du renvoi introuvable.**) can only take place if the mass goes above or below the storage limit defined in the** Erreur ! Source du renvoi introuvable..

If the modification of the mass occurs after these 7 days following the initial entry then the storage number is modified only when the mass value falls to zero mg.

Of course in both cases the unique number attached to the product does not vary and remains the reference to use.

As an administrator, you can also reassign this product to another chemist by clicking on “reassign the structure to another chemist” (Picture 28)



Picture 28 *: modification of a file*

You then arrive on a page (Image 29) which allows you to choose the new chemist by selecting his team then his manager in the drop-down menus on the left of the screen or by directly entering the first letters of his name in the box " name of chemist. Once the chemist is selected, click on to perform the backup.

Image 29: reassignment of a structure to a chemist

3. Search all free and patented data

The "Search" section of the left "Menu" (Image 69) allows the user to carry out a search according to various criteria in all the free and patented substances in the laboratory's Chemical Library.

Substances under contract appear only for the owners (*chemist, manager and leader)* of that substance.

Anyone can search by structure (exact, substructure or similarity), molar mass, raw formula, tags and numbering. For the latter, you can use either the unique random 8-digit number, or the number defined in the "product parameters" section (example: ICOA-FST-L-01A02 see Chapter ID1), or the number of the National Chemical Library (CN000000V) if it was imported by the administrator, or by the QR-code.

For molar mass and crude formula, you can perform an exact search by checking the "exact" box. Otherwise, by default you search by pattern.

Image 30: search form

Once the search criteria has been entered and the “Search” button has been clicked, the results page appears. The presentation is similar to the “modification” section (chapter I.B.2.b)), but with only the possibility of consulting the substances. The consultation sheet only contains the “structure” and “Analysis” tabs.

4. Biological results

This menu tab is reserved for user types: **managers** and **bosses** . It allows them to consult, for each biological test carried out, the results on their substances. These results must first have been imported by the administrator (see Chapter **Erreur ! Source du renvoi introuvable.**).

The user must first select the target, the type of biological test and finally the type of result (IC50, % activity, etc.). The user can visualize the molecules involved in the biological test and the corresponding results (Image 31).

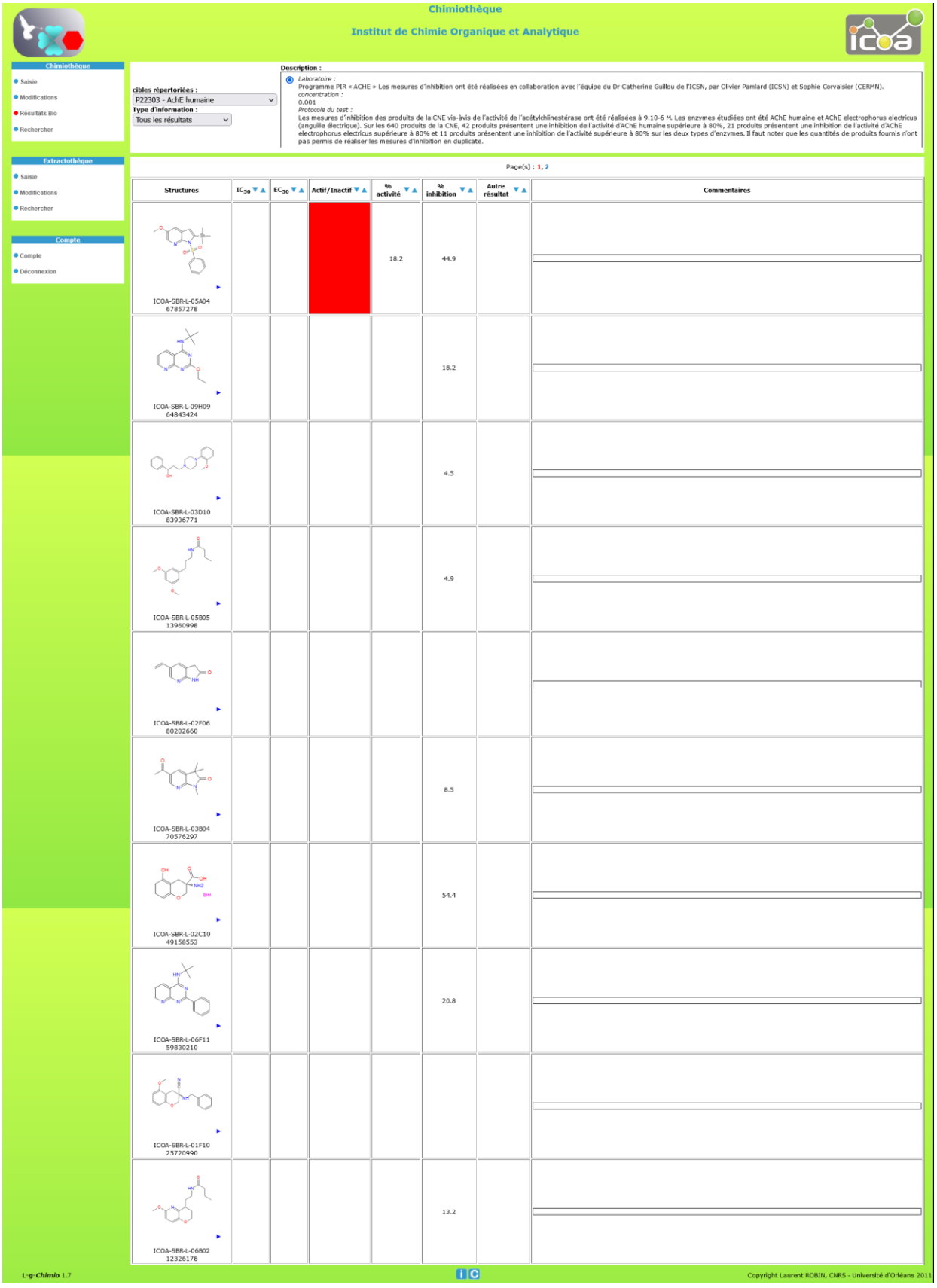


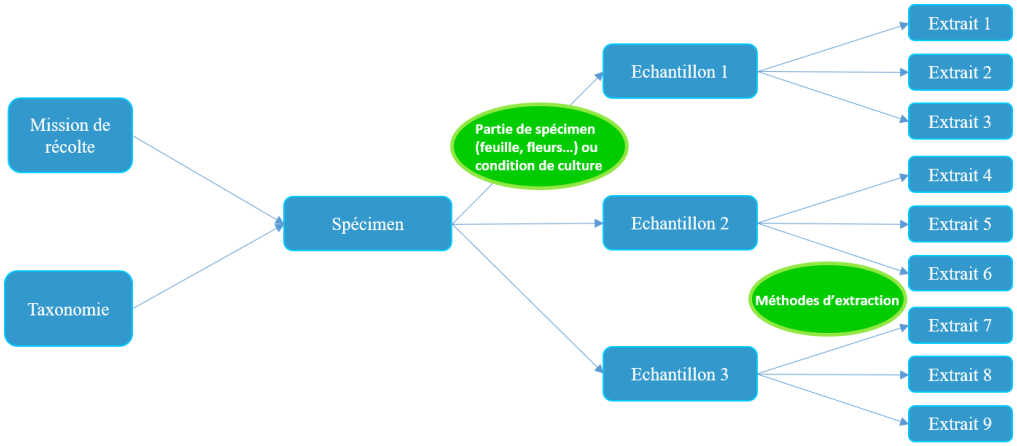
Image 31: Biological result for a team's molecules for a chosen biological test

C. Extract Library Part

1. Entering a new extract

a) Direct entry via the entry tab

To enter a new extract, go to the “Extract library” menu and select the “entry” tab. You then arrive on a page showing the architecture of the database (Picture 32)



Picture 32 *: data architecture*

An **extract** is linked to a sample which is itself linked to a specimen.

A **specimen** is described by the “harvesting mission” table and the “taxonomy” table. As a reminder, a specimen is an individual(s) (plant, insect, microorganism, etc.) from which the sample is obtained; it is defined by its genus and species name.

The **sample** corresponds to the entire specimen or part of a specimen (leaves, bark, venom, etc.) or to a specimen of the microorganism type obtained under certain culture conditions, it is from the sample that the we prepare the extract.

Please note: The *Country* , *taxonomy type* and *part of organization fields* must have been completed in the “Administration” menu, “Extract library / Parameters” tab before starting to enter an extract.

To save a new extract, you must select “extract” in the drop-down menu at the location “I want to enter a:” (Image 33)

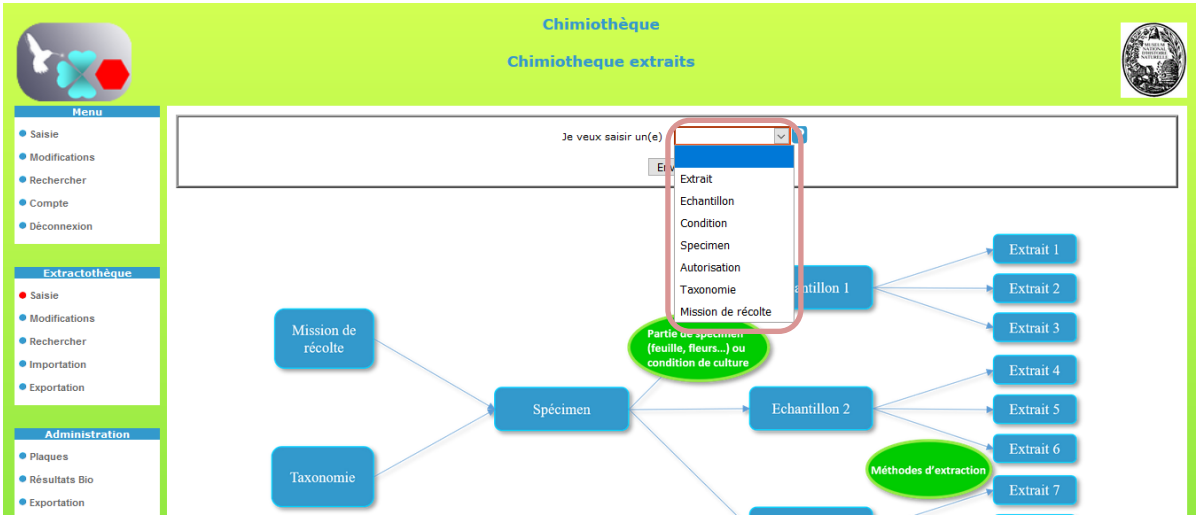


Image 33*: drop-down menu to enter a new extract*

Then click send. A list of questions will then appear to which you must answer yes or no.

“Does the sample exist? » :

- If you answer "yes" because the sample is already saved in the database, you have one more step to save your extract. To do this, click on the “Step 1: Extract” banner, and refer to the chapter STEP 7: Extract
- If you answer "no" because the sample is not saved in the database, you get two more questions: "Do you want to create a new condition?" » and “Is the specimen extant?” ".

“Do you want to create a new condition?” » :

- If the specimen is not a microorganism (bacteria, microscopic fungus, etc.), you must answer “no” to this question.
- If your specimen is a microorganism and the culture protocol has never been described in the database, you must answer “yes” to create a new condition (=culture protocol). If the protocol used has already been recorded in the database for another specimen, you must answer “no” and will be asked to select the existing protocol in the database in a future step.

“Is the specimen extant?” » :

- If you answer “yes”, you have 2 steps left to save your extract. To do this, click on the “Step 1: Sample” banner, and refer to the STEP 6: Sample.
- If you answer "no" because the specimen is not registered in the database, you arrive at three more questions: "Is authorization required?" », “Does the taxonomy exist? » and “Does the harvest mission exist? ". After answering these questions, you must also complete the “Specimen” table, refer to the STEP 4: Specimen.

“Is authorization necessary? »:

- You must answer “yes” if your specimen is subject to the Nagoya protocol.

The so-called principle of access and benefit-sharing (ABS) is established by the Convention on Biological Diversity and the Nagoya Protocol. It implies that access to genetic resources and their use are subject to an agreement between the supplier and the user of the resource.

- An intermediate question then appears: “Does the authorization exist?” ", i.e. is it already recorded in the database? If yes, you move on to the next question. If the answer is no, in the next step you will need to record the authorization number (APA Permit No., sample collection authorization, sampling permit, etc.) See STEP 3: Authorization

“Does the taxonomy exist? »:

- If you answer “yes”, it means that you are working on a specimen different from that recorded either due to its geographical origin, or due to the season in which it was collected, or on a plant part different from that already recorded or either because you are working on a microorganism obtained in culture conditions different from those recorded... But most often the answer will be “no” and you will then have to complete the “taxonomy” table See STEP 2: Taxonomy

“Does the harvest mission exist? »:

- If you answer “yes”, because the mission during which the specimen was collected has already been registered on the database, you have 4 steps left to register your extract starting with step 1: “Taxonomy”. To do this, click on the “Step 1: Taxonomy” banner, and refer to the STEP 2: Taxonomy
- If you answer "no", you have 5 steps left to save your clip. To do this, click on the “Step 1: Harvest mission” banner, and refer to the chapter STEP 1: Harvest mission.

the records already present in the database using the help placed opposite.

Only certain fields are mandatory fields and must be completed to allow you to proceed to the next step. They are marked with a * and a red frame. The other fields are optional fields.

(1) STEP 1: Harvest mission

Complete the fields then click on send, only the *Country field* is a required field. You must use the drop-down menu to fill in this field (Image 34)

Please note: The *Country field* must have been entered in the “Administration” menu, “Extract library and settings” tab before starting the entry. To do this, use the official country reference https://documentation.abes.fr/sudoc/formats/CodesPays.htm

Image 34*: drop-down menu of countries*

(2) STEP 2: Taxonomy

Complete the fields then click on send, only the *Type* , *Species* and *Genus fields* are required fields. The *Type* field must be selected from the drop-down menu (Image 35)

Please note: The *Type field* must have been entered in the "Administration" menu, "Extract library and parameters" tab before starting the entry.

In the *sequencing field* , you can note the sequenced genome (for example: 18s), complete the sequencing *protocol and attach the result file by clicking on browse.*

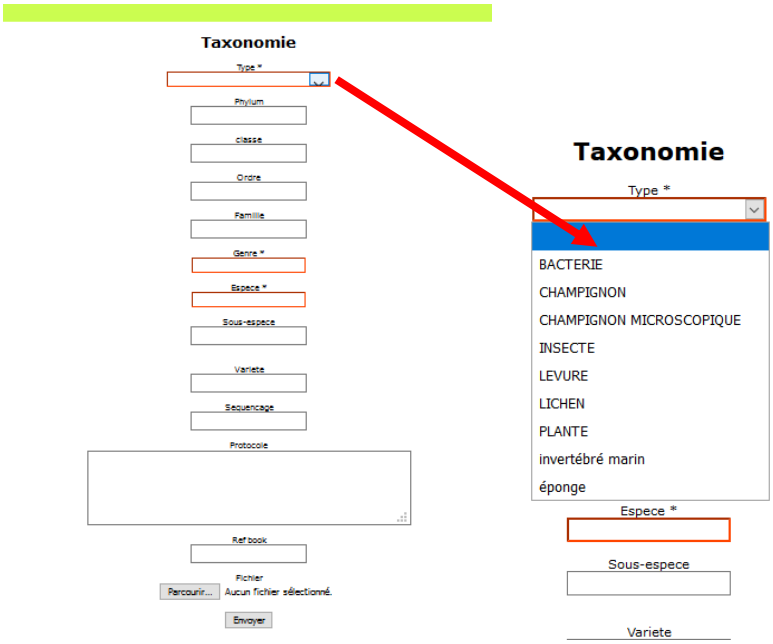


Image 35*: Taxonomy Type drop-down menu*

(3) STEP 3: Authorization

No fields are required at this stage. The *type of authorization* can be for example: APA permit, direct debit authorization, etc. Complete the fields then click on send.

Image 36*: Taxonomy Type drop-down menu*

(4) STEP 4: Specimen

Entry into the " *Specimen" table* is done in 4 phases:

- In the 1st phase , only the specimen *code , date* and *place of collection fields* marked with an * are mandatory. At this stage, information can be added on the collection (GPS coordinates, name of the collector, etc.) or on the collection from which the specimen came. You can also click on "browse" and add a photo (Image 37)

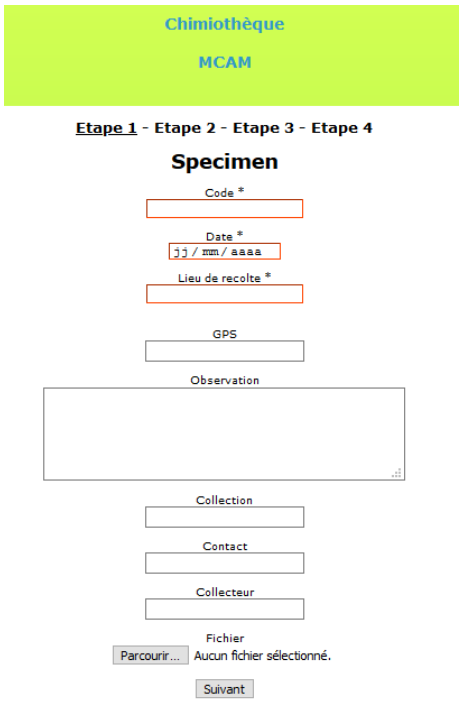


Image 37*: Specimen entry drop-down menu*

- In phase 2, you must attach an authorization to the specimen (see Nagoya protocol – APA). If no authorization is required, leave no check mark and proceed to the next step.
- In phase 3 you must attach a taxonomy to the specimen. You can make your search easier by sorting the genus or species name by column. Select the corresponding line and click next.
- You arrive at phase 4 where you will associate a collection mission with the specimen. Sort columns by mission name or country code to make your search easier.

Then click send.

(5) STEP 5: Condition (only if your specimen is a microorganism)

In this step you will have to describe the culture conditions of the microorganism by completing the table below, only the *temperature field* is a mandatory field (Image 38)

Image 38*: description of culture conditions for a microorganism*

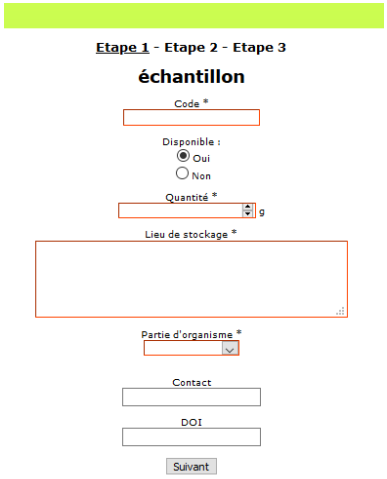
If the culture conditions have already been saved in the database, you will need to attach them to the *specimen* in the next step.

(6) STEP 6: Sample

Filling the "Sample *" table* is done in 3 phases:

- In the 1st phase , only the *code* , *quantity* , *storage location fields* and *part of organism* are obligatory (Picture 39).

Please note: The *Part of organization field* must have been entered in the "Administration" menu, "Extract library/parameters" tab before starting the entry.



Picture 39 *: 1st phase of filling for the sample*

- The 2nd phase consists of attaching a condition (culture protocol) to the specimen. You can make your search easier by sorting the information by column. Select the corresponding line and click next.

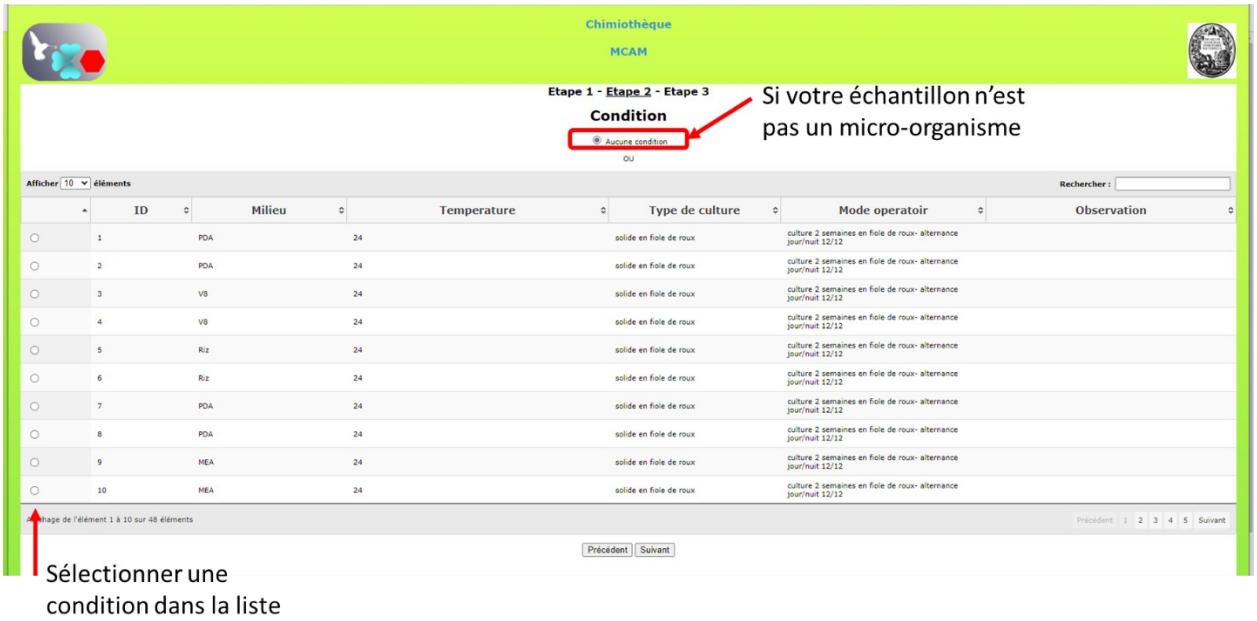
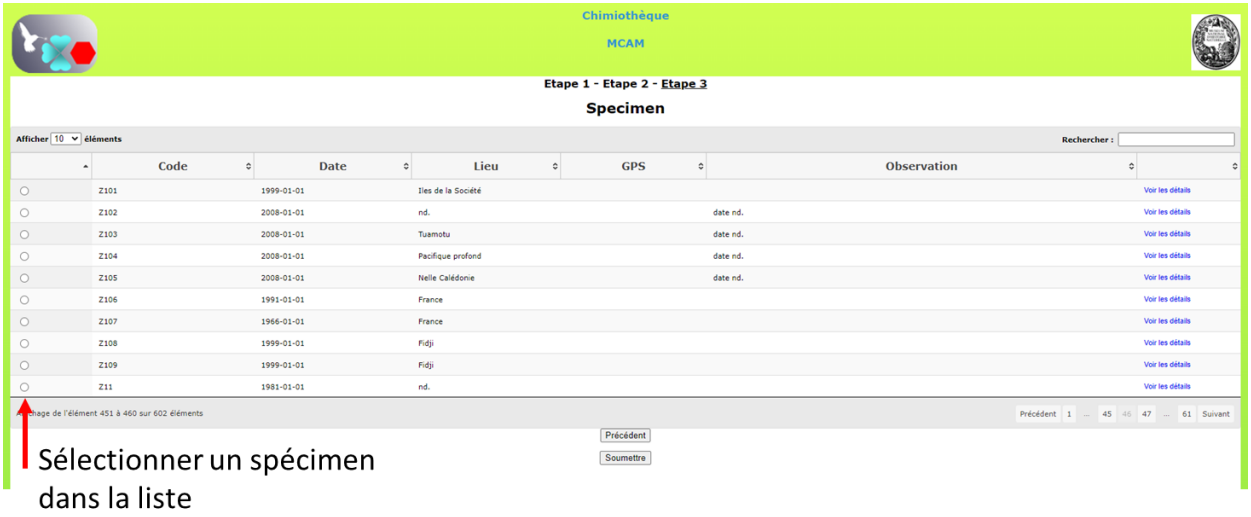


Image 40*: 2nd phase, conditions*

Warning: If your sample is not a microorganism, you do not have any conditions to attach to it and you must select "No conditions".

- You then arrive at the 3rd phase corresponding to the specimen table. Select a specimen from the list. You can facilitate your search by sorting by column the code of the specimen, its place of collection... Select the corresponding line and click on submit (Picture 41)



Picture 41 : *table of specimens*

(7) STEP 7: Extract

The entry into the "Extract" table is done in 3 phases:

- the 1st phase covers the extraction protocol and the characteristics of the extract. It is at this stage that the code of the extract is determined (Cf. chemical librarian's manual, chap.7 "product coding"). Fields marked with * are mandatory fields, other fields are optional. Drop-down menus or examples are offered at each step in the help (Picture 42). For the *chemist name field* , you have a drop-down menu with the names of chemists already saved in the database. If the chemist is not yet registered, you must create an account for him beforehand (see: **Erreur ! Source du renvoi introuvable.**). You can select the extraction solvent using the drop-down menu provided.

Picture 42 : *First phase*

- The 2nd phase corresponds to the type of purification carried out on the extract, select "None" if nothing has been carried out on the extract.

- The 3rd phase allows you to attach the sample to your extract. To find the sample, you can use the “search” function located at the top right, or sort the columns by code. By default, the license type is “free”.
  Click submit. The home page reloads with the message “The entry procedure is finished”.

Your extract is saved!

b) Import via a csv format file

This method is the fastest if you need to record several extracts at the same time. It is preferred for new users, because it is simpler to implement.

The csv file is made up of several tables:

- the Extract table
- the Sample table
- the Specimen table
- the Taxonomy table
- the Shipping table
- the Chemist table
- the Condition table (optional table)

In each table there are several fields, mandatory fields and optional fields. You can find the list of fields in the **importation_Extrait-2.csv file** . This file is available in the Extract library menu, import tab by clicking on “explanation and example for import” (Picture 43)

Picture 43 *: import tab*

The csv file template is shown below (Image 44), this file contains all the fields available in the database. Not all of these fields need to be completed, only a few fields are mandatory and marked in green in the csv file. Fields in orange are optional fields.

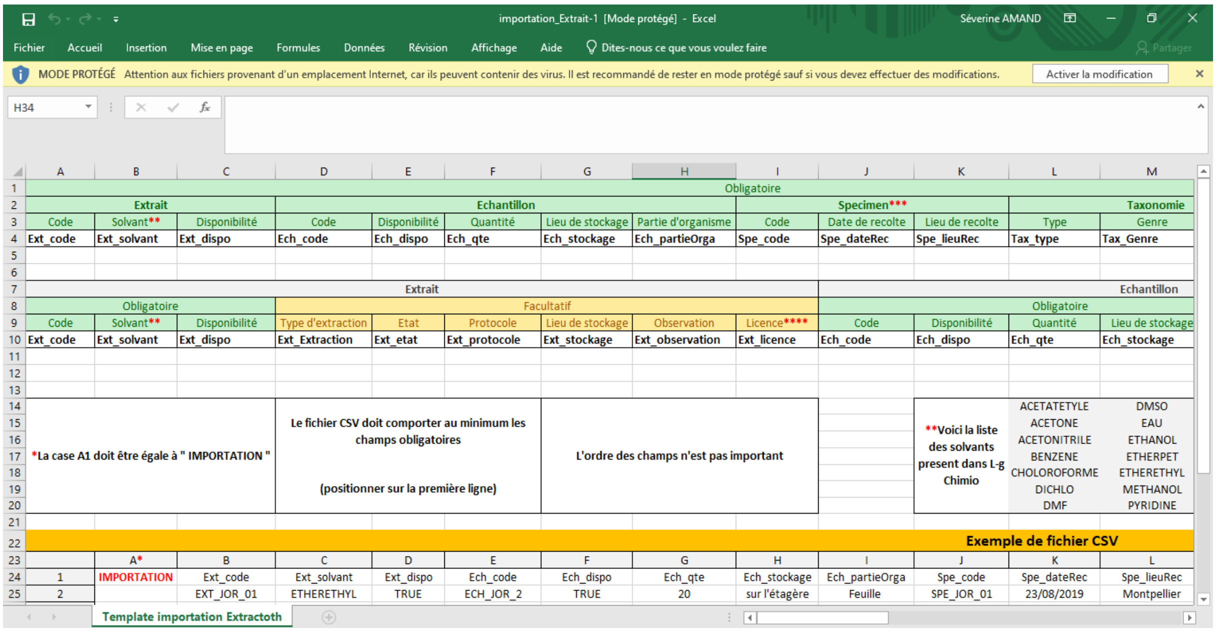


Image 44: csv file for data import

To fill the *Ext_solvent field* you must refer to the glossary for this field (Picture 45)

**Voici la liste des solvants present dans L-g Chimio				Si le solvants n'est pas present dans la liste, il sera automatiquement remplacer par " INCONNU "
	ACETATETYLE	DMSO	THF	
	ACETONE	EAU	TOLUENE	
	ACETONITRILE	ETHANOL	INSOLUBLE	
	BENZENE	ETHERPET	INCONNU	
	CHOLOROFORME	ETHERETHYL		
	DICHLO	METHANOL		
	DMF	PYRIDINE		

Picture 45 : *glossary of the Ext_solvent field*

To fill in the *Exp_country* field you only need to note the country code.

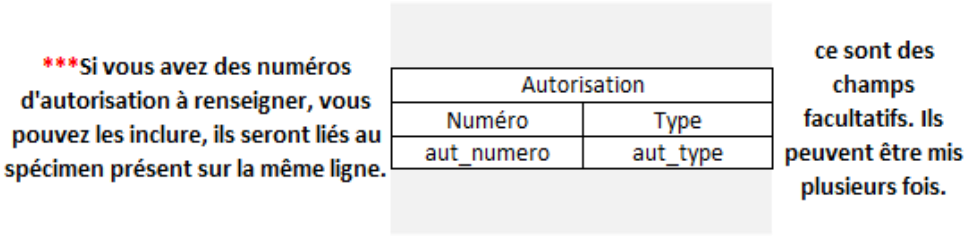
Warning: To allow the data to be imported correctly, box A1 of the file must be equal to IMPORT. The order of the fields in the file is not important, but the file must contain at least all mandatory fields, i.e. 16 fields. The country code must be saved in the software before importing.

To fill in the optional *Ext_licence field* you must use the lexicon (Image 46).

****Liste des types de licences dans L-g Chimio		Si le type n'est pas présent dans la liste, il sera automatiquement remplacé par " LIBRE "
	LIBRE	
	CONTRAT	
	BREVET	

Image 46: *glossary of the Ext_licence field*

If you have collection authorizations for some of your specimens (APA, etc.) you must enter them using the *aut_numero fields* and *aut_type* (Picture 47)



Picture 47 : *Added authorization for the specimen table*

Here is an example of a completed file ready to be imported (Picture 48). The file must be imported in csv format.

	A	B	C	D	E	F	G	H	I	J
1	IMPORTATION	Exp_pays	Tax_phylum	Tax_classe	Tax_Ordre	Tax_famille	Tax_type	Tax_Genre	Tax_Espece	Spe_code
2		FR	Basidiomyco	Basidiomyce	Agaricales	Agaricaceae	champignon	Agaricus	arvensis	MIC-001
3		FR	Basidiomyco	Basidiomyce	Agaricales	Agaricaceae	champignon	Agaricus	radicatus	MIC-002
4		FR	Basidiomyco	Basidiomyce	Agaricales	Bolbitiaceae	champignon	Agrocybe	praecox	MIC-003
5		FR	Ascomycota	Pezizomycet	Pezizales	Pyrenemata	champignon	Aleuria	versicolor	MIC-004
6		FR	Basidiomyco	Basidiomyce	Agaricales	Pluteaceae	champignon	Amanita	echinoeocep	MIC-005

K	L	N	P	Q	R	S	T	U	W
Spe_dateRe	Spe_lieuRec	Spe_collecti	Spe_collecte	Ech_code	Ech_dispo	Ech_stockag	Ech_partieO	Ech_contact	chi_nom
01/01/2008	France	Champignon	D. Michelot	MIC-001-1	oui	spécimen da	entier	Amand / Ma	Roland Lupoli
27/10/1986	France	Champignon	D. Michelot	MIC-002-1	oui	spécimen da	entier	Amand / Ma	Roland Lupoli
05/06/1986	France	Champignon	D. Michelot	MIC-003-1	oui	spécimen da	entier	Amand / Ma	Roland Lupoli
22/05/1986	France	Champignon	D. Michelot	MIC-004-1	oui	spécimen da	entier	Amand / Ma	Roland Lupoli
23/09/1986	France	Champignon	D. Michelot	MIC-005-1	oui	spécimen da	entier	Amand / Ma	Roland Lupoli

U	W	X	Y	Z	AA	AB	AC	AD	AE
Ech_contact	chi_nom	Ext_code	Ext_solvant	Ext_dispo	Ext_Extraction	Ext_etat	Ext_protocol	Ext_stockage	Ext_observation
Amand / Ma	Roland Lupoli	MNHN-CX-0001	METHANOL	oui	agitation	en solution c	agitation per	congélateur	2 plaques 96 puits
Amand / Ma	Roland Lupoli	MNHN-CX-0002	METHANOL	oui	agitation	en solution c	agitation per	congélateur	2 plaques 96 puits
Amand / Ma	Roland Lupoli	MNHN-CX-0003	METHANOL	oui	agitation	en solution c	agitation per	congélateur	2 plaques 96 puits
Amand / Ma	Roland Lupoli	MNHN-CX-0004	METHANOL	oui	agitation	en solution c	agitation per	congélateur	2 plaques 96 puits
Amand / Ma	Roland Lupoli	MNHN-CX-0005	METHANOL	oui	agitation	en solution c	agitation per	congélateur	2 plaques 96 puits

Picture 48 : *example of csv import file*

To import the csv file, go to the “Extract library” menu and select the “import” tab then select the file to import using the “browse” function then click on send.

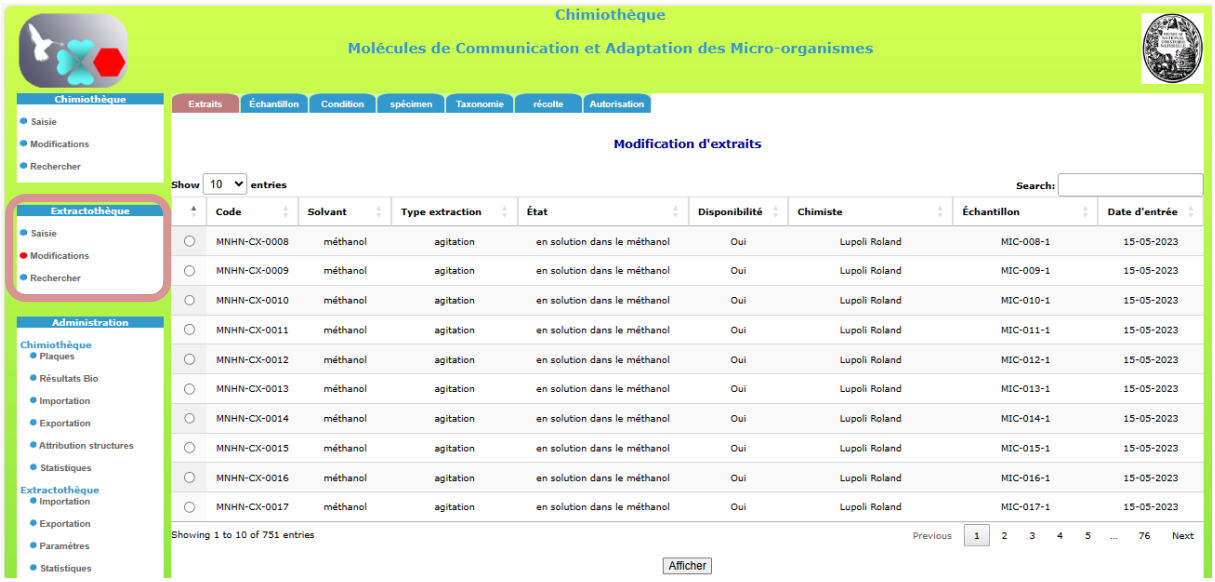
Please note: The *Country* , *taxonomy type* and *part of organization fields* must have been entered in the “Administration” menu, “Extract library/parameters” tab before importing the csv file.

The software then displays the message “import completed, number of lines read: xx” to indicate that the import was successful.

2. Editing and viewing an extract

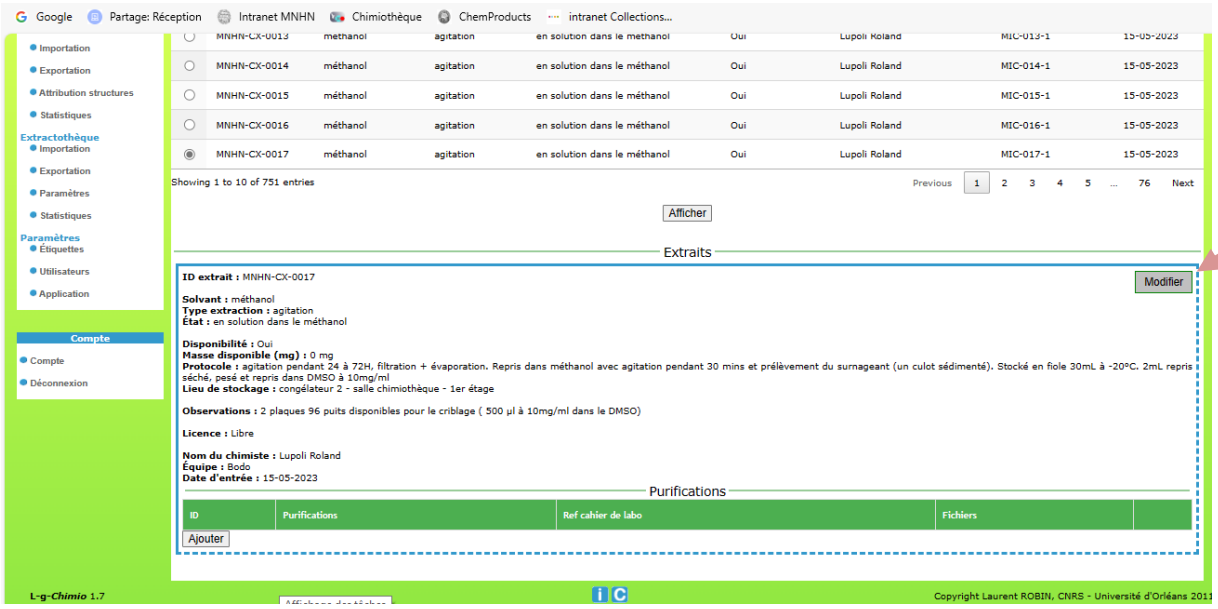
a) Editing an extract

Go to the “Modification” tab of the “Extract Library” menu. This function allows you to modify any field. It can be useful for updating the quantities of extract or samples available.



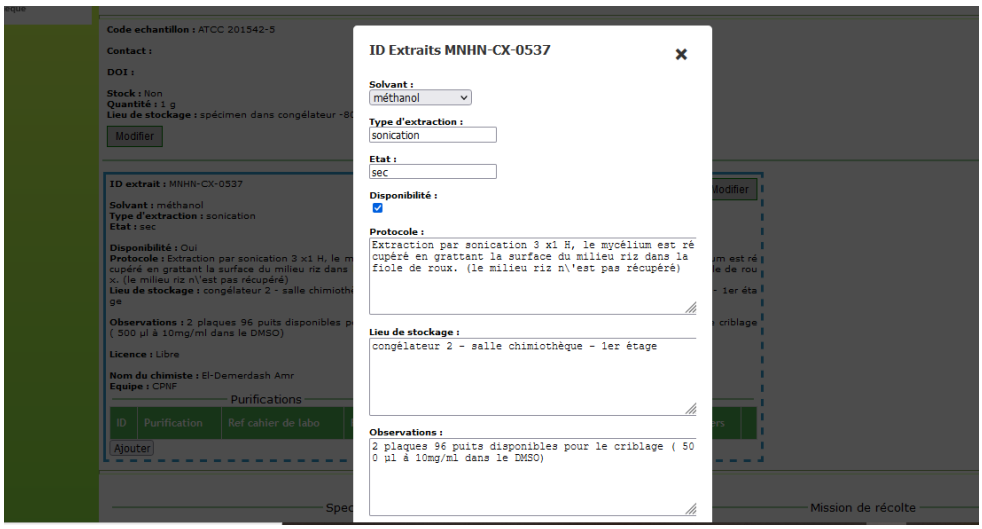
Picture 49 *: edit page*

You can go to the tabs in any table and sort the columns alphabetically or use the search function at the top right to select an extract or specimen… Click search at the bottom of the screen, the selected extract (specimen…) appears, you can then click at the top right of the table on the modify function.



Picture 50 *: location of the modify button*

You access a window where all the editable fields are present. Click on modify to validate the modification.

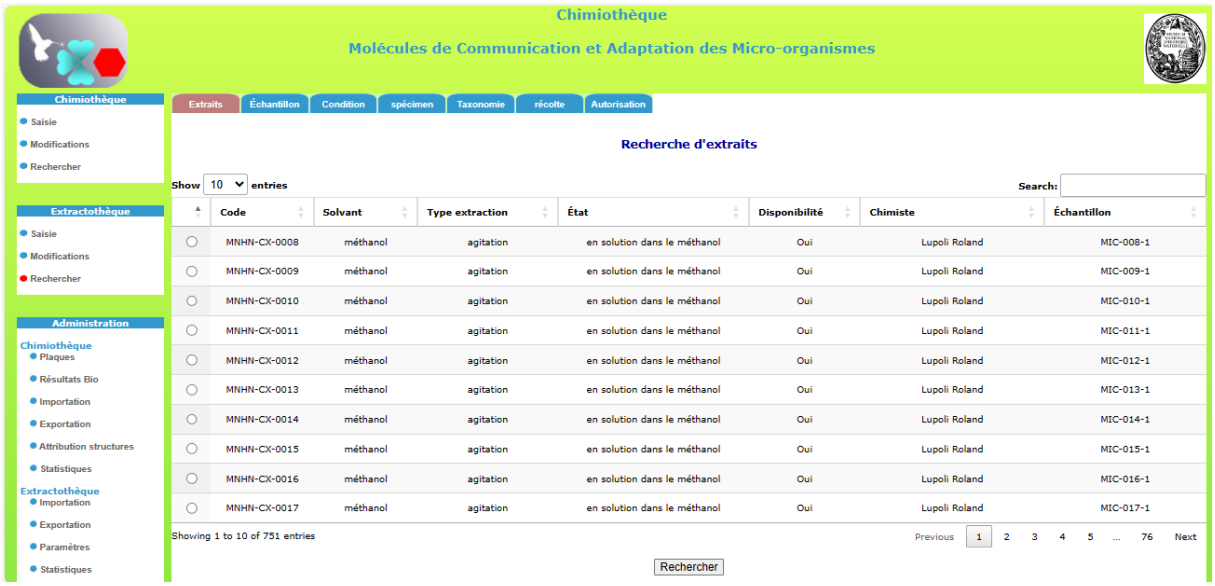


Picture 51 : *edit page*

b) Research

Go to the “search” tab in the “Extract library” menu. The search is in the form of a tab allowing you to search for either an extract, a sample, a specimen, or a taxonomy.

In each tab you can then sort the columns alphabetically or use the search function at the top right.

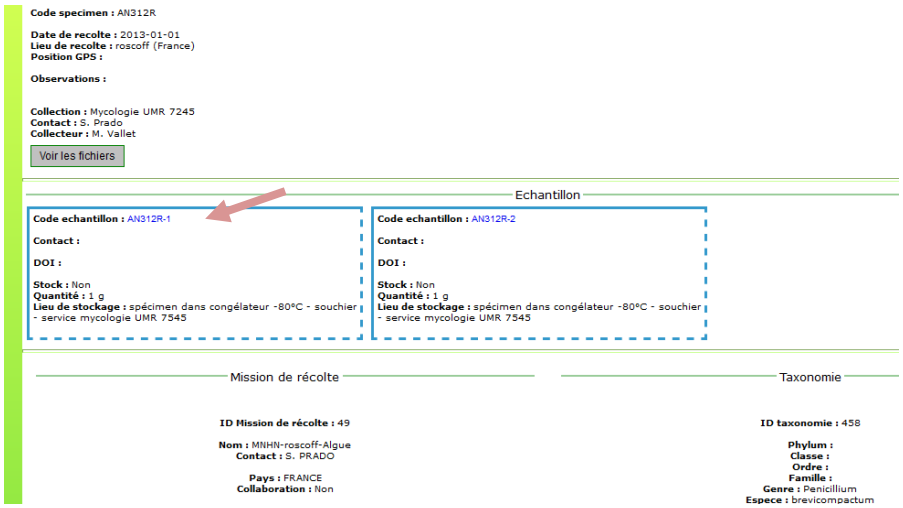


Picture 52 : *view of the Search page*

Select the desired row and click search at the bottom of the window.

For an extract, a window appears at the bottom of the page with the extract information. If you want to access the corresponding sample click on “ view sample ”. Several windows are displayed below the first, which contain all the information.

For a specimen, in the same way, you can click on the sample code (in blue) to access this information.



Picture 53 *: localization of the sample code*

Certain tabs (harvesting mission, authorization, etc.) do not allow a precise search , but only to view the data recorded in the database.

D. Account settings

Each user can modify their account settings (Image 54). He can change the email address, the language of the account *(French or English)* or even modify his password.

For the administrator(s), manager(s), manager(s), the option of activating or deactivating the return by email each time one of its users enters is possible.

Each manager receives, if the option is activated here, an email each time one of the users of his team enters, the leader will have all the users of the teams attached to him.

The administrator receives an email for all user entries.

Each user can choose the interface language, either French (fr) or English (us).

Each user can change the password that was automatically assigned to them. The new password must be a minimum length of 12 characters.

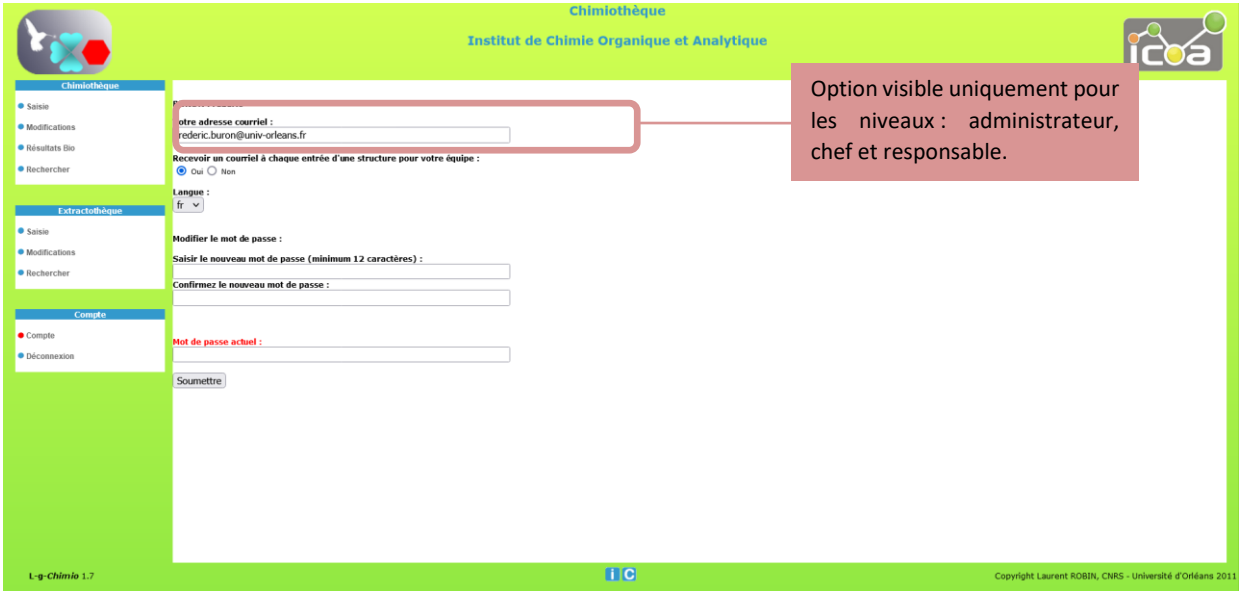


Image 54: Account settings page

E. FAQs

The analysis file downloaded during entry does not appear when viewing the file:

This type of problem comes from the PHP settings. In the PHP configuration, edit the php.ini file (for a Linux distribution go to the /etc directory. Look for the “memory_limit” and “post_max_size” parameters and increase their respective value so that it is representative of all the data posted by the user for entering a molecules file If the user loads 4 files of 10M each into a file, plus the data in text form, these parameters must therefore be at least equal to 50M. : post_max_size = 50M, memory_limit=50M.

II. Appendices

A. Recommendations for standardizing NC structures

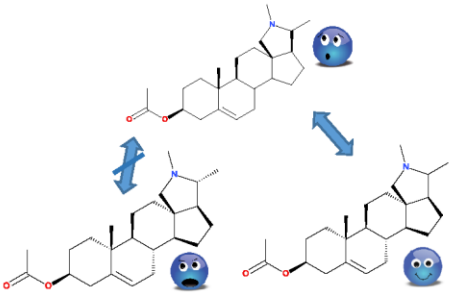
Université de Strasbourg

cnrs

Recommendations for the standardization of structures of the National Chemical Library

F. Ruggiu, G. Marcou, D. Horvath, A. Varnek
Laboratoire d'Infochimie, Université de Strasbourg
E. Grand
Laboratoire des Glucides, Université de Picardie
F. Massicot
Université de Reims-Champagne-Ardenne

This document summarizes recommendations for representing the structures of substances referenced in the National Chemical Library in order to reduce the number of ambiguities that hinder the automatic processing of data and the interpretation of screening results.

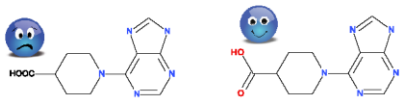


1

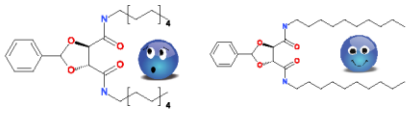
Format and identifier

Check before transmitting structures that the identifiers are in accordance with the National Chemical Library.
Use the SDF v2000 format. The fourth line of the file must end with V2000. Some tools like ChemDraw automatically save in SDF v3000 if elements not supported by the v2000 format are introduced in the drawing. In this case, it is necessary either to redo a saving by eliminating these components (often chemical groupings, labels, colors, geometrical shapes), or to use a third party tool to make the conversion.

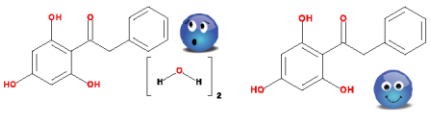
Implicit/explicit groups



Do not use an implicit representation of chemical groups.



Do not use shortened notations.

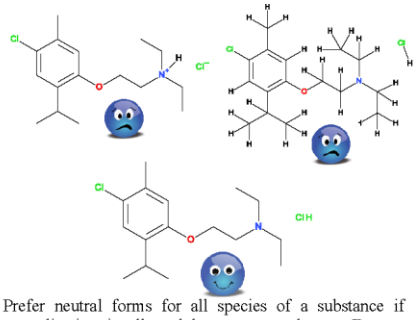


Note on configuration : H2O=2

Do not represent water molecules for a hydrate and specify the degree of hydration d in the Note on configuration field using the syntax H2O=*d*.

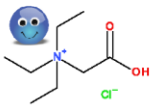
2

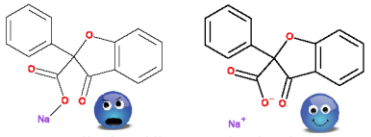
Hydrogens and formal charges



Prefer neutral forms for all species of a substance if neutralization is allowed by proton exchange. Do not represent hydrogens explicitly. Implicit hydrogens are deduced from the valence state and formal charge.

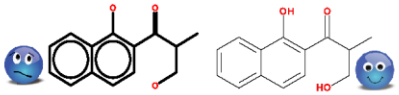
Formal charges are shown when they are permanent. The necessary counter ions are not neutralized.





Do not neutralize by adding a covalent bond.

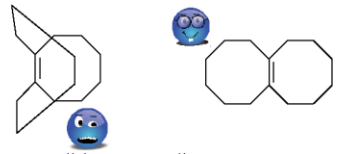
Aromatizations



The kekulized forms of the cycles are always preferred.

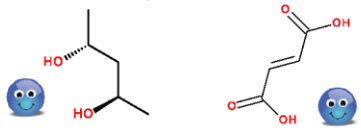
3

Crossings



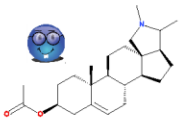
Do not cross links unnecessarily.

Stereochemistry

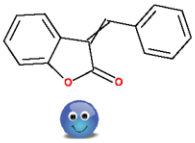


The absolute configuration of the stereogenic centers is specified by the orientation of the bonds extending from them. The "corner" of a stereo bond must be on the side of the asymmetric atom.

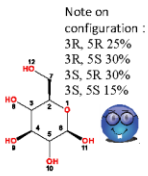
If the configuration of one or more stereogenic centers is not specified, this indicates that the substance is stereochemically pure, but the isolated stereoisomer is not known.



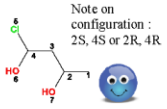
If the stereoisomericity of a double bond is represented by a Cis/Trans double bond it means that a stereoisomer is isolated, but it is not known which one it is.

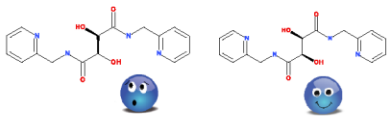


If more than one stereoisomer is present in the solution: use an atom numbering to specify the proportions of the stereoisomers in the Note on the database configuration field. Racemates are a special case of this situation.

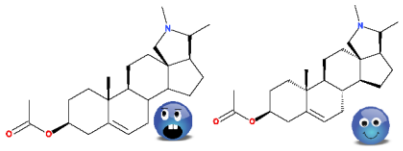


If the substance contains the drawn compound or its enantiomer, the enantiomeric pair is specified in the Note on configuration field.

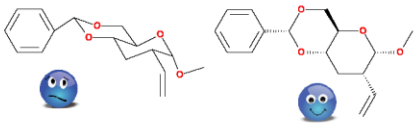




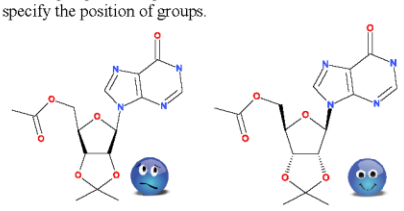
Two asymmetric atoms must not be connected by a stereo bond.



Specify the stereochemistry of all asymmetric centers explicitly, especially if it is implicit as, for example, for the frames gonane, estane, androstane, pregane and their alkenes.

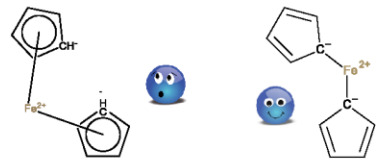


Pseudo-perspective representations should not be used to specify the position of groups.



Do not use specific representations (Haworth, Fisher,...) to specify the stereochemistry.

Organometallics



Prefer representations using covalent bonds in compliance with the Lewis rules. Only conventional bonds (single, double, triple and aromatic) are supported by all electronic formats used in the databases.