2024

L-g-Chimio V1.7



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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 <u>Image 1</u>) 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 (<u>Image 2</u>). Otherwise, you return to authentication, with the possibility of requesting a password again (<u>Image 3</u>) by clicking on the link "Lost password" see chapter: I.A.2.



Image 1: Login to the application



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 (<u>Image 4</u>) 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.

	Formation chimiothécaires et extractothécaires ChemBio France	e
Connexion Nom :	Nom :	
Connexion	Votre adresse courriel :	
Perdu le mot de passe ?	Soumettre	

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 ($\underline{\text{Image}}$ $\underline{5}$), 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.

Chimiothèque 6 Saisie 9 Modifications 9 Rechercher	Chimiothèque Formation chimiothécaires et extractothécaires $\bigcirc \square \times $	ChemBisFrar	nce
Extractothèque Saisie Modifications Rechercher Administration Chimiothèque Plaques Résultats Bio Importation Exportation Attribution structures Statistiques	N O S F F C I Br I P X X	* : champ obligatoire nom du chimiste : Nom Prenom Origine de la molécule : - Sélectionnez une origine - V Etape de synthèse de la molécule : Sélectionnez une étape - V * Masse de produit disponible : mg V Type de structure : Libre V	Champ apparaissant uniquement pour le(s) administrateur(s) et chef(s)
Encontration Exportation Exportation Paramètres Statistiques Paramètres Etiquettes Utilisateurs Application Compte Compte Déconnexion	JSME Molecular Editor by Peter Ertl and Bruno Bienfait JME : Aide Recommandations pour le dessin des structures Note sur la configuration :		Soumettre

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" (<u>Image 6</u>). 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.

ile	Edit	Options	Object	Chem	istry Window	Help										
⊜Tra	2	Undo	Ctrl+Z	101	🖌 📄 🔲 Atal			→ 10	• B	/ <u>U</u> ≡	33	"C + CH	x ² X ₂	ا لا	🖉 🖄 🖽	-
	64	Redo	Ctrl+Y													
۶ 4	est :	Cut	Ctrl+X	×1.	1 1 1 1 1	11	/ 0	🕈 🕛 🖸 M	0 5 1	H F	CI Br	I B	K A	۹	• 🔺	
20	1	Сору	Ctrl+C													
÷.		Paste	Ctrl+V													
•		Copy As			Molfile Ctrl+M											
•		Paste Text /	As 🕨		SMILES String											
*		Duplicate	Ctrl+D		NEMA Key	- 1										
)		Delete	Suppr		Chimestring	- 1										
1		Italic	Ctrl+I		Sketch String	- 1										
•		Bold	Ctrl+B		InChl String	- 1										
1		Underline	Ctrl+U		InChl Key	- 1										
,c		Select All	Ctrl+A		IUPAC Name											
•		Insert Ohie	ct	-	Sequence Text	- 1										
- 1	-			- 1	Bitmap	- 1										
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•																

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).

Paste	×
Paste the text to import into the text area below. Or drag and drop a file on it.	
Accept Parcourir Aucun fichier sélectionné. Cancel	

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 Omg. 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 <u>Image 8</u>.



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 <u>Image 9</u>.

	Chimiothèque	
	Institut de Chimie Organique et Analytique	
	Chimiothèque	
Saisie		
Modifications		
Rechercher		
	Extractothèque	
Saisie		
Modifications		
Rechercher		
	Attention doubion I La structure existe dejà dans la base. Voulez-vous continuer ?	
Chimiothèque Plaques		
Résultats Bio	OK Annuler	
Importation		
•		

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 <u>Figure 10</u>. 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.

	c Institut de Chin	Chimiothèque nie Organique et Analytique	ic a
Chimiothèque • Saisie	= : champ obligatoire	Numéro de pilulier : ICOA-IGU-L-08C10	
Subin Modifications Rechercher Extractothègee Salaie Modifications Rechercher	Q	Code(c)-harre(c) au Qecode(c)) ; (séparts par un retour à la ligne) * Masse de produit disponible : 9 0 0 m mg	Solvants de solubilisation : cettes d'éthyle secteme secteme beruisee d'ethersonnelle d'ethersonnelle personnelle d'ethersonnelle personnelle secteme secteme beruisee d'ethersonnelle personnelle secteme beruisee d'ethersonnelle personnelle secteme beruisee d'ethersonnelle secteme beruisee secteme beruisee secteme beruisee secteme beruisee secteme beruisee secteme beruisee secteme beruisee secteme beruisee secteme beruisee secteme beruisee secteme beruisee secteme beruisee secteme beruisee secteme beruisee beruisee secteme beruisee secteme secteme beruisee secteme secteme beruisee secteme beruisee secteme s
Administration Chaministration Programs ® Resultate Bo ® Reportation © Exportation © Adminutores © Satistrapues	С с с с с с с с с с с с с с с с с с с с	Type de purification : - Sélectionnez une purification - • Aspect : - Sélectionnez Taspect - • Précautions à prendre stocker sous argon se dégrade solde éférence cabier de laboratoire ou theise :	PHILO enu
Importation Exportation Paramètres Paramètres Paramètres Paramètres Paramètres Utilisateurs Auptication	Nom en nomencleture IUPAC (angleise) :	Node operatore : Analyses	
Compte © Compte © Déconnexion	Analyse ôfômentaire :		
	Point d'ébuilition : ~c A pression de : atm	Point d'ébuilition	
	Pureté mesurée : 16 % Méthode de mesure de la pureté :	Pureté de la sabstance mesare de l'4 _D	
	es Température : [™] C [™] C	сси :	
	Rf : Solvants utilisés :		
	spectrométria UV	spectrométrie	lafaranga
	Fichier du spectre UV : Parcourit / Aucun fichier sélectionné. Spectrométrie de Masse	Fichier du spectre IR : Parcourir Aucun fichier sélectionné. Spectrométrie de Mass	se haute résolution
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	Source of Leakables : → Selectiones & Source → → Fickler du sector SH : Parcouric., Aucun ficher sélectionné. Sourtematrice BHN ⁵ M	Source d'Industition : 	. рын ¹³ г
	opectionnoise dans in	Données RMM ¹² C :	
	Fichier du spectre RNN ² H : Parcourit Aucun fichier sélectionné.	Fichier du spectre RNN ¹³ C : Parcouric Aucun fichier sélectionné. Bibliographie & Observations -	
	Bibliographie	Observations	
	Publication numéro IDOT : numéro INAL :	Upper values :	
	Référence CAS :		Crampeters .
L-g-Chimio 1.7			Copyright Laurent ROBIN, CNRS - Université d'Orléans 2011

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 (CN00000V) 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* (<u>Image 12</u>)

The chemist (<u>Image 12</u>) 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 (<u>Image 14</u>) 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 .

Lg-Chemo 2024

Chimiothèque	
• Saisie Ánuines :	
● Modifications type de molécule : Sélectionnez une équipe マ	
Rechercher	
Sélectionnez un collaborateur 💙	Partie propre
Extractothèque	א chaque type
	d'utilisateur
	u utilibuteur
Rechercher C	
Administration 0 Masse molaire en g.mol ⁻¹ :	
Chimiothèque S	
• Plaques ou ou	
Résultats Bio	
Importation	
Exportation	
• Attribution structure:	Partie
Statistiques	commune
Extractothèque Importation I	commune
• Exportation ou	
Paramètres Péférence cabler de laboratoire ou thèse :	
Statistiques	
Paramètres	
Etiquettes JSME Molecular Editor by Peter Erti and Bruno Bienfait	
Utilisateurs JME: Ade	
• Application	
Compte Recurrence par: © structure exacte O sous structure O Similante - Coefficient de similante : min 0 max 1 valeur: 0.6	
Compte Recher lier	
Déconnexion	
L-g-Chimio 1.7 Copyright Laurent ROBIN, CNRS - Université d'Orléans 2011	

Image 11: search page seen by the administrator

	Chimiothèque	
	Insutut de Chinne Organique et Anaryuque	icoa
Chimiothèque		
Modifications	type de molécule : Sélectionnez le type ¥	Rechercher
Rechercher		
Extractothique Saisie I Modifications Recharcher Compte Compte Compte Compte	Name Name <th></th>	
	JSME Molecular Editor by Peter Eril and Brunno Biernfast Tag de la structure : 	Berburbar
L-g-Chimio 1.7	li C	Copyright Laurent ROBIN, CNRS - Université d'Orléans 201:

Image 12: Display seen by the chemist guy

		Chimiothèque	
	Institu	t de Chimie Organique et Analytique	icoa
Chimiothèque			
Saisie	type de molécule :	collaborateurs :	Rechercher
 Modifications 	Sélectionnez le type V	Sélectionnez un collaborateur V	No. Recitorer
Résultats Bio			
Rechercher		Masse molaire en g.mol ⁻¹ :	
Extractothèque	c	= V	
• Saisie	N	ou	
Modifications	0	Formula hauta :	
Rechercher	F	exacte	
		ou	
Compte		Numérotation :	
• Compte	P	2	
Deconnexion	x	ou	
		Référence cahier de laboratoire ou thèse :	
		ou	
	JSME Molecular Editor by Peter Ertl and Bruno Bienfait	GAVO	
	JME : Aide	v	
	Bacharchar par : Structure exacts Sour structure Sour structure	te eimiladhá - min 0 may 1 yalaur: 0.6	
	Source per . O source course of sous of source of similarite - Coefficient	A ANNOLO A A VAIGUE UND	
			Rechercher
L-g-Chimio 1.7			Copyright Laurent ROBIN, CNRS - Université d'Orléans 201

Image 13: Display seen by the responsible guy

	Institut (Chimiothèque de Chimie Organique et Analytique	îcoa
Chimiothèque Saisie Modifications Résultats Bio Rechercher	type de molécule : 	équipes : - Sélectionnez une équipe - ∨ ou cuitaborateurs : - Sélectionnez un collaborateur - ∨	Rechercher
Lstractothique Satue Modifications Katelencher Compte Compte Decompte Decompte	Image: Second	Hasse molaire en g.mor ¹ : ou i'ormale brute : ou Numérolation : ou Référence cahier de laboratoire ou thèse : ou Référence cahier de laboratoire ou thèse : ou sérilanté : min 0 max 1 valeur: 8.6	
			Rechercher
L-g-Chimio 1.7			Copyright Laurent ROBIN, CNRS - Université d'Orléans 2011

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 (<u>Erreur ! Source du renvoi</u> 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 (<u>Image 15</u>).



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** (<u>Image 16</u>)



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. Rightclick on the structure, you obtain a menu (<u>Image 17</u>).



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 sin the search results page, you access the consultation of the substance sheet. This is modulated according to the user's rights.

Structure 🚺 Analyses 🛛 Résultats Bio 🗍 Historique

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.



<u>Image</u> 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 (<u>https://fr.wikipedia.org/wiki/Digital Object Identifier</u>),
 - the CAS number (<u>https://fr.wikipedia.org/wiki/Num%C3%A9ro_CAS</u>),
 - the HAL number (<u>https://fr.wikipedia.org/wiki/HAL (archive ouverte)</u>)
- 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.

	Chimiothèque						
	Institut de (Chimie Organique et Ana	alytique	icoa			
Chimiothèque	Structure Analyses						
• Saisie	Nom :						
Modifications	Phenyl-6-(4-methoxyphenyl)-3,4-dihydropyrid						
Rechercher	Structure contrôlée : Non contrôlée		Numéro : ICOA-IGU-L-04E07				
	Pureté contrôle : Non contrôlée Date contrôle pureté :		Numéro constant: 18346758				
Extractothèque			Numéro Chimiothèque Nationale :				
Saisie	\sim		Code barre/Qrcode :				
Modifications			Date d'entrée : 2012-03-09 11:02:13				
Rechercher			Couleur du produit : #FFFFFF				
			Masse molaire : 309.359 g.mol ⁻¹				
Compto			Masse de produit disponible : 5 mg				
Compte			Tare du pilulier : 0 mg				
Compte			Present en plaque(s) : Non				
Deconnexion			Nem : Nicolae (FGANT				
	Note sur la configuration :		Origine de la molécule : Synthèse				
	Mode opératoire :		Type du produit : Libre				
	Sous atmosphère inerte, une solution de 50 mg de phosphate vinylique x (0.11 mmol, 1		Etape de synthèse : Inconnue				
	dégazée trois fois avant d'être agitée pendant 15 minutes. 31 mg (0.14 mmol, 1.25 éq.)		Aspect du produit : solide				
	de dioxazaborocane, 0.17 mL d'une solution aqueuse de Na2CO3 2M (0.33 mmol, 3 éq.), 0.25 mL d'eau et quelques gouttes d'EtOH sont ajoutées au milieu réactionnel avant		Logp : 3.84				
	d'être porté à reflux pendant 90 minutes. Après refroidissement, la solution est filtrée sur célite et rincée à l'AcOEt et à l'eau. La phase aqueuse est extraite à l'AcOEt, puis les		Vérifie les règles de Lipinski : oui Analyse élèmentaire théorique : C(72 77%) N(0.00%) C(15 52%) N(6 19%)				
	phases organiques sont lavées avec une solution aqueuse saturée en NaCl, séchées sur MoSO4, filtrées et concentrées. Une chromatographie sur gel de silice (éluant : EP/écOEt.		Analyse élèmentaire expérimentale :				
	95/5 à 8/2) permet d'isoler le composé x (24 mg, 71%) sous forme d'un solide blanc.		Type de purification : colonne				
			Référence du cahier de laboratoire : NG376				
	Observations :		Nombre d'accepteurs : 3				
			Nombre de liaisons rotatives: 4				
			Nombre de liaisons aromatiques : 12				
			Nombre de donneurs : 0				
			Nombre d'atomes asymétriques : 0				
			Point de fusion : 96 Point d'ébulition :				
			Précaution(s) :				
			Solvant(s) : acétate d'éthyle, acétone, chloroforme, dichlorométhane, THF,				
	numéro DOI :	Référence CAS :	numéro HAL :				
L-g-Chimio 1.7			Copyright Laurent R	DBIN, CNRS - Université d'Orléans 2011			
	Image 10): "Structure" ta	h				
	image 12	. structure tu					

(2) "Analysis" tab

In the "Analysis" tab (<u>Image 20</u>), 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.

		Chimiothèque	
	Institut de	Chimie Organique et Analytique	icoa
Chimiothèque	Structure Analyses		
Saisie Medificatione	Pureté mesurée : %		
Rechercher	Méthode de mesure de la pureté :		
Extractothèque	spectrométrie UV :		
• Saisio			
Modifications			
Rechercher			
Compte			
Compte			
Déconnexion	Enastromátria da Massa :		
	2021-11-29		
	SM (IS): m/z = 310.0 [M+H]+.		
	Source d'ionisation : INCONNU		
	Spectrométrie de Masse haute résolution :		
	Source d'ionisation :		
	RMN ¹ H : 2021-11-29		
	RMN 1H (CDCl3, 400 MHz): 📓 (ppm): 1.98 (qt, 2H, H3, J = 6.8 Hz), 3.33 (qt, 2H, H4, J =		
	3.8 Hz), 3.79 (s, 3H, OCH3), 3.85 (q, 2H, H2, J = 5.4 Hz), 5.42 (t, 1H, H5, J = 3.8 Hz), 6.79 (d, 2H, Har, J = 6.2 Hz), 6.85 (d, 2H, Har, J = 8.8 Hz), 7.06 (t, 1H, Har, J = 7.5 Hz), 7.20 (d, Hz), Hz = 0.0 Hz), 0.0 Hz =		
	1H, Haç J = 8.0 Hz), 7.23 (d, 1H, Har, J = 7.6 Hz), 7.32 (d, 2H, Har, J = 8.8 Hz).		
	RMN ¹³ C : 2021-11-29		
	RMN 13C (CDCI3, 100 MHz): 圓 (ppm): 23.7 (1ÍCH2, C4), 23.9 (1ÍCH2, C3), 45.7 (1ÍCH2,		
	(C2), 55.5 (11CH; 50CH3), 113.8 (21CH; CarH), 115.7 (11CH; C5), 121.5 (21CH; CarH), 125.4 (11CH; CarH), 126.4 (21CH; CarH), 129.2 (21CH; CarH), 132.6 (CIV; Car), 139.5 (CIV; Car), 151.2 (CIV; Car; Qu C=Q), 153.5 (CIV; Car; Qu C=Q), 159.1 (CIV; Car).		
	an ataon itala Kafananan a		
	2021-11-29		
	IR (pur): 圓 (cm-1): 2928 (CH), 2837 (CH), 1701 (C=O), 1638 (C=C), 1608 (C=C), 1511		
	(C=C), 1193 (C-O).		
	a 🗅 :		
	a Température : a Concentration :		
	a Solvant :		
	Rf : 0.57		
	CCM Solvants utilisés : EP/AcOEt : 8/2		
L-g-Chimio 1.7		Copyright Laurent ROBIN	, CNRS - Université d'Orléans 201

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 (<u>Image 21</u>). A result only appears if it was imported by the administrator using the import tools (see: Chapter **Erreur ! Source du renvoi introuvable.**).

							Chimioth	èque				
					Insti	tut de C	himie Orga	nique et Ana	lytique			îcoa
Chimiothèque	Structure	Analyses	Résultats Bio	Historique								
 Saisie 			Cible			Actif		· · · · · · · · · · · · · · · · · · ·	Résultats			Commentaires
Modifications			Choice				% d'activité	% inhibition	IC ₅₀ en nM	EC ₅₀ en nM	Autre résultat	
Rechercher	AchE humaine	22303						12.8				
Extractothèque Saisie Modifications					Páfárar		iProt					
Rechercher					Referen	ice on	IPTOL					
Noom de la cil Chinathipue Paques Résultats Bo Résultats Bo Exportation Statistiques Exportation Exportation Paramètres Statistiques Paramètres Composition Paramètres Composition Paramètres Composition Paramètres Par	ble											
Compte												
Compte												
Déconnexion												
L-g-Chimio 1.7							iC	3				Copyright Laurent ROBIN, CNRS - Université d'Orléans 2011

Image 21: "Organic results" tab

By hovering over the name of the biological test, you access the details (<u>Image 22</u>). The number next to the name of the biological test here P22303 on Image <u>Image 22</u>it is the UniProt reference (<u>https://fr.wikipedia.org/wiki/UniProt</u>) 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 (<u>Image 23</u>). 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.

	Chimiothèque Institut de Chimie Organique et Analytique								
Chimiothèque	Structure Analyse	s Résultats Bio Historique							
• Saisie			Modifications effects	iées sur cette fiche					
Modifications			riouncations critica						
Rechercher	Qui robin Laurant	Date de la modification	Champs Nom :	Ancienne valeur					
	robin Laurent	2018-05-22 17:17:45	Structure	WVFWOMXBQG0GBD-UHFFFAOYSA-N					
Extractothèque	robin Laurent	2018-05-22 17:17:46	Type de purification :	colonne					
Saisie	robin Laurent	2018-05-22 17:17:46	Aspect du produit :	huile					
Modifications	robin Laurent	2018-05-22 17:17:46	a Solvant :	Aucune valeur Ancient uméro unique : 2222152					
Rechercher	robin Laurent	2018-05-22 17:17:46	Etape de synthèse :	Inconnue					
Administration									
Chimiothèque Plaques									
Résultats Bio									
 Importation 									
Exportation									
Attribution structures									
Statistiques									
Extractothèque Importation									
Exportation									
Paramètres									
Statistiques									
Paramètres • Étiquettes									
 Utilisateurs 									
 Application 									
Compte									
 Compte 									
Déconnexion									
L-g-Chimio 1.7			i C		Copyright Laurent ROBIN, CNRS - Université d'Orléans 2011				

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.

						ILUJ
Chimlothèque	Il y a 12975 réponse(s) répartie(s) sur 1622 p	age(s)	page 1	page 2		Aller à la page
Saisie						
Modifications						
Rechercher						
Extractothèque		ICOA-FST-L-01A02 : 311mg PAVE Grégoire 20-12-2001 Responsable : Franck SUZENET pureté contrôlée : Non contrôlée	~		ICOA-FST-L-01A03 : 73mg PAVE Grégoire 03-01-2002 Responsable : Franck SUZENET pureté contrôlée : Non contrôlée structure contrôlée : Non contrôlée	2
Modifications	ОН	Exportation				
Rechercher			×			
		Tout copier da	ans le presse papier			
			Ou			
Chimiothèque Plaques				•		
Résultats Bio	C ₁₀ O ₃ H ₈	Expor	rter la page	g.mol ⁻¹		
Importation	170.109 (Linut -					
Exportation						
Attribution structures	Ĩ	ICOA-FST-L-01A04 : 36mg PAVE Grégoire 08-01-2002			ICOA-FST-L-01A05 : 96mg Alphonse France-Aimée 08-01-2002	
Statistiques		Responsable : Franck SUZENET Surveté contrôlée : Non contrôlée			Responsable : Franck SUZENET pureté contrôlée : Non contrôlée	
Extractothèque Temportation	ОН	structure contrôlée : Non contrôlée	_N ▼	\square	structure contrôlée : Non contrôlée	
Exportation						
Paramètres	X		N*			

Image 25: Choice between the 2 export options

	Il y a 12975 réponse(s) répartie(s) sur 1622 page(s)		page 1			
Modifications						
Recharcher						
Estavetothiopen Salasie Modifications Recharcher		PST-L-01402 : 313mg maabate : Prants 5023mit extended : Prants 5023mit extended : State : Stat	×0. ×			
		Tout copier dans le presse papier				
Administration in 11		⊕ localhost		* 1		
Résultata filo		la liste a été copier l				
• Importation		-	ок			
• Exportance						
Statistrypen						
Extractolhèque Importation						
Exportation						

Image 26: Copying the list to the clipboard

	Chimiothèque	
	Institut de Chimie Organique et Analytique	ເດືອ
Chimiothèque	EXPORT CSV	
Saisie		
Modifications		
Beshereber		
• Rechercher	Séléctionnez les champs à exporter :	
	Selectionnez les champs souhaitè V	
Extractothèque	Sélectionnez vos critères de sélection :	
Saisie	Equipe	
mouncations		
 Rechercher 		
	Produits en plaque mais pas en vrac	
Administration	Produit chez EVOTEC mais plus en vrac	
	Тад	
Chimiothèque Plaques		
	Seulement les produits presents crez evoie:	
 Resultats Bio 	Les deux	
 Importation 		
Exportation	Depuis une liste o loentilicateurs	
Attribution structures	Liste d'identificateurs :	
Autouton structures	ICOA-FST-L-01A02;ICOA-FST-L-01A03;ICOA-FST-L-01A04;ICOA-FST-L-01A05;ICOA-FST- L-01A05;ICOA-FST-L-01A02;ICOA-FST-L-01A04;ICOA-FST-L-01A05;ICOA-FST-	
 Statistiques 	L-01400,1004-000-2.1004-001-0-01402,1004-001-0-01403	
Extractothèque		
Importation		
Exportation		
Paramètres		
Statistiques	Séparateur utilisé pour la liste :	
Paramètres Étiquettes		
	Not de passe :	
Utilisateurs	Mot de passe	
 Application 		
Compte		
Compto		
Compte		
 Déconnexion 		
L-g-Chimio 1.7		Copyright Laurent ROBIN, CNRS - Université d'Orléans 2011

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" (<u>Picture 28</u>)

	Molécules de Communicat	Chumotheque ion et Adaptation des Micro-organismes	
Chimiothèque			Réattribuer la structure à un autre chimiste
• saise			P
Modifications			
Saisie Modifications Recharcher	index of the output of th	una un Tag – v) u v	
Administration Chimiothèque P Rejout Résultats Ello e Importation e Exportation e Athlohoin structures	Etape de synthése de la malée "Hasse de produit dispondité X X A A A A A A A A A A A A A	de ; <u>fiscentus</u> ♥ de 5 <u>mg</u> ♥ ♥ e cruitede ♥ a et valide ♥ a+c4-21	
Statistiques	Insoluble chez Evotec 7 🗆		
Extractothèque Importation Exportation	► ME_Ade		
Paramétres	Recommendations over la descia des advertants		
Paramèteer	Note sur la configuration :		
Eliquettes			
Utilisateurs			Soumettre
Application			
Comete			
Compte			
Déconnexion			
L-g-Chimio 1.7		fic (opyright Laurent ROBIN, CNRS - Université d'Orléans 20:

Picture 28 : modification of a file

You then arrive on a page (<u>Image 29</u>) 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 a to perform the backup.

L	Molécules de Communi	Chimotheque cation et Adaptation des Micro-organismes		
Source Conversion Research on the Conversio		Attribution de structure MNHN-CH-0561 Recher	cher -	
International Control of Control	Filiptioner and and figure () . Opportunities of the second of the seco	B	ean de charactes ; Du Burson défer	
L-g-Chimio 1.7		IIC	Copyright Laurent ROBIN, CNRS - Université	d'Orléans 20

Image 29: reassignment of a structure to a chemist

3. Search all free and patented data

The "Search" section of the left "Menu" (<u>Image 69</u>) 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 (CN00000V) 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.

		Chimiothèque	
	Institut	t de Chimie Organique et Analytique	້ເວັ້ອ
Chimiothèque			
• Saisie	;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;		
 Modifications 		Masse molaire en g.mol ⁻¹ :	
Rechercher	C		
Extractathàqua	N O	ou	
Saisia	s	Formule brute :	
Modifications	F	i exacte	
Rechercher	CI	ou	
- Hecherener	Br	Numérotation ·	
Administration	P		
Chimiothèque Plagues	x	ou	
Résultats Bio		Référence cahier de laboratoire ou thèse :	
Importation			
Exportation		ou	
Attribution structures		Tag de la structure :	
Statistiques	JSME Molecular Editor by Peter Ertl and Bruno Bienfait	GAVO	
Extractothèque	JME : Alde	~	
Exportation			
Paramètres	Bacharchar par : Structure exacte Sous structure Similarité - Coefficient d	ta similaritá - min 0 may 1 valeur: 0.6	
 Statistiques 		A STUBALLE : HULLO	Deckarder
Paramètres • Étiquettes			Recifer citer
Utilisateurs			
Application			
Compte			
Compte			
Déconnexion			
L-g-Chimio 1.7		fi C	Copyright Laurent ROBIN, CNRS - Université d'Orléans 2011

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 (<u>Image 31</u>).

						Chimioth	èque				
	Institut de Chimie Organique et Analytique										
Saisie	cibles répertoriées :		Descript O Lai Pro	ion : boratoire : ogramme PIR « ACHE	» Les mesures	d'inhibition ont été	réalisées en colla	boration avec l'équipe du Dr Catherine Guillou de l'ICSN, par Olivier Pamlard (ICSN) et Sophie Corvaisier (CERMN).			
Modifications Résultats Bio	P22303 - AchE humaine V Cool P22303 - AchE humaine V Cool Potocole du test : Protocole du test : Trave, key feathers V Les ensures difficibilities del a CNE vis-àvis de l'activité d										
Rechercher			(ar ele pa	nguille électrique). Su ectrophorus electricus s permis de réaliser l	r les 640 produi supérieure à 8 es mesures d'ini	its de la CNE, 42 p 0% et 11 produits hibition en duplicat	a vue rowno vue vacume ou aconynommesorase on eve reasses a 3 v10- PL Les enzymes etudees ont été ACIE: humàine et ACIE étotophorus electricus de la CIE, 42 produits présentem une inhibition de l'activité supérieure à 80%, sur les deux types d'enzymes. Il faut noter que les quantiés de produits forsient de la mérit, al produits présentem une inhibition de l'activité supérieure à 80% sur les deux types d'enzymes. Il faut noter que les quantiés de produits forsient don en duplicax.				
Extractothèque							Page(s)	: 1,2			
Modifications	Structures	IC ₅₀ ▼ ▲	EC ₅₀ ▼ ▲	Actif/Inactif 🔻 🔺	% activité ▼▲	% inhibition * •	Autre résultat 🔻 🔺	Commentaires			
Rechercher	- 0										
Compte Compte	or po				18.2	44.9					
Déconnexion	<u> </u>										
	ICOA-SBR-L-05A04 67857278										
	~~										
						18.2					
	64843424										
	90.0										
	de la companya de la comp					4.5					
	ICOA-SBR-L-03D10 83936771										
	" Å										
						4.9		[]			
	•										
	ICOA-SBR-L-05805 13960998										
	NH NH							·۱			
	LCOA-SBR-L-02F06 80202660										
	i.										
						8.5					
	LCOA-SBR-L-03B04 70576297										
	он g										
						54.4					
	ICOA-SBR-L-02C10 49158553										
						20.8					
	•										
	ICOA-SBR-L-06F11 59830210										
	to										
	ICOA-SBR-L-01F10										
	25720990										
						13.2					
	ICOA-SBR-L-06802 12326178										
L-g-Chimio 1.7				<u>n</u>		ic	3	Copyright Laurent ROBIN, CNRS - Université d'Orléans 201			

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 (<u>Picture 32</u>)



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 (<u>Image 34</u>)

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

	and the second se						
	Chimiotheque						
	МСАМ						
Mission de récolte							
Nom							
	Contact						
	Pays * (Voir les détails des pays)						
	ANTARTIQUE						
	ARGENTINE						
	AUSTRALIE						
	BENIN						
	BRESIL						
	CANADA						
	CONGO						
	CHINE						
	CURACAO						
	DIBOUTI						

(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 (<u>Image 35</u>)

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.

Chimiothèque MCAM	
Autorisation	
Numéro d'autorisation	
Type d'autorisation	
Envoyer	
Image 36: Taxonomy Type drop-down m	enu

(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 (<u>Image 37</u>)

Chimiothèque
МСАМ
<u>Etape 1</u> - Etape 2 - Etape 3 - Etape 4
Specimen
Code *
Date * jj/mm/aaaa
Lieu de recolte *
GPS
Observation
Collection
Contact
Collecteur
Fichier Parcourir Aucun fichier sélectionné.
Suivant

Image 37: Specimen entry drop-down menu

- In phase 2, you must attach an authorization to the specimen (<u>see Nagoya protocol APA</u>). 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 (<u>Image 38</u>)

Chimiothèque
Chimiotheque extraits
Condition
conation
Milieu
Temperature * C
Type de culture
Mode opératoire
Observation
Choisir des fichiers Aucun fichier n'a été sélectionné
Soumettre

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.



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 (<u>Picture 39</u>).

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.

2					Chimiothèqu MCAM						
				Eta	pe 1 - <u>Etape 2</u> - I Condition Aucure condition OU	Etape 3	Si vo pas u	tre échantillor un micro-orgar	n n'est nisme		
Afficher	10 🗸 élémen	ts								Rechercher :	
	•	ID ≎	Milieu 0	Temperature	о Туј	e de culture	0	Mode operatoir	0	Observation	0
	1	PDA	24		solide en fiole	de roux	culture jour/n	e 2 semaines en fiole de roux- alternance uit 12/12			
0	2	PDA	24		solide en fiole	de roux	culture jour/n	e 2 semaines en fiole de roux- alternance uit 12/12			
	3	V8	24		solide en fiole	de roux	culture jour/n	e 2 semaines en fiole de roux- alternance uit 12/12			
0	4	VS	24		solide en fiole	de roux	culture jour/n	e 2 semaines en fiole de roux- alternance uit 12/12			
0	5	Riz	24		solide en fiole	de roux	culture jour/n	e 2 semaines en fiole de roux- alternance uit 12/12			
0	6	Riz	24		solide en fiole	de roux	culture jour/n	e 2 semaines en fiole de roux- alternance uit 12/12			
	7	PDA	24		solide en fiole	de roux	culture jour/n	e 2 semaines en fiole de roux- alternance uit 12/12			
0	8	PDA	24		solide en fiole	de roux	culture jour/n	e 2 semaines en fiole de roux- alternance uit 12/12			
	9	MEA	24		solide en fiole	de roux	culture jour/n	e 2 semaines en fiole de roux- alternance uit 12/12			
0	10	MEA	24		solide en fiole	de roux	culture jour/n	e 2 semaines en fiole de roux- alternance uit 12/12			
Ahage	de l'élément 1 à	10 sur 48 éléments								Précédent 1 2 3	4 5 Suivant
					Précédent Suivan	t					
S	électio	onner une									
С	onditi	on dans la l	iste								

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 (<u>Picture 41</u>)

						No. 1
			Etap	pe 1 - Etape 2 - <u>Etape 3</u>		
				Specimen		
er 10 🗸 é	éléments					Rechercher :
	Code	≎ Date	≎ Lieu ≎	GPS ≎	Observation	\$
	Z101	1999-01-01	Iles de la Société			Voir les détails
	Z102	2008-01-01	nd.	date nd.		Voir les détails
	Z103	2008-01-01	Tuamotu	date nd.		Voir les détails
	Z104	2008-01-01	Pacifique profond	date nd.		Voir les détails
	Z105	2008-01-01	Nelle Calédonie	date nd.		Voir les détails
	Z106	1991-01-01	France			Voir les détails
	Z107	1966-01-01	France			Voir les détails
	Z108	1999-01-01	Fidji			Voir les détails
	Z109	1999-01-01	Fidji			Voir les détails
	Z11	1981-01-01	nd.			Voir les détails
ge de l'élém	ent 451 à 460 sur 602 éléments				Précé	dent 1 45 46 47 61 5
				Précédent		

- 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 ? (<u>Picture 42</u>). 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" (<u>Picture 43</u>)

	Chimiothèque	a.
	Molécules de Communication et Adaptation des Micro-organismes	
Chimiothèque		
Saisie	Importation pour l'extractothèque	
Modifications		
Rechercher		
Extractothèque	Taille maximum du fichier 128M	
Saisie	Choisir un fichier Aucun fichier n'a été sélectionné	
 Modifications 		
Rechercher	Explication et exemple pour l'importation	
Administration	Soumettre	
Chimiothèque Plaques		
 Résultats Bio 		
 Importation 		
 Exportation 		
 Attribution structures 		
 Statistiques 		
Extractothèque Importation		
Exportation		

Picture 43 : import tab

The csv file template is shown below (<u>Image 44</u>), 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.

i	🕁 🕤 🖑 🕫 importation_Extrait-1 (Mode protégé) - Excel Séverine AMAND 🗷 – 🗗 🗙													
Fic	hier Accu	ueil Insertion	Mise en page	Formules Donn	iées Révisio	n Affichage	Aide 🛛 Dites-	nous ce que vous vou	lez faire					
6	MODE PRO	DTÉGÉ Attention	aux fichiers provenan	t d'un emplacement	Internet, car ils p	peuvent contenir de	s virus. Il est recomm	nandé de rester en moi	de protégé sauf si	vous devez effectuer	des modifications.	Activer la m	odification	×
-														
Ha	4		Ĵ _X											1
			-	-		-	-							
1	A	В	С	D	E	F	G	н	hligatoiro	J	K	L	м	H
2		Extrait				Echantillon		0	ligatone	Specimen***			Taxonomie	
3	Code	Solvant**	Disponibilité	Code	Disponibilité	Quantité	Lieu de stockage	Partie d'organisme	Code	Date de recolte	Lieu de recolte	Type	Genre	1
4	Ext_code	Ext_solvant	Ext_dispo	Ech_code	Ech_dispo	Ech_qte	Ech_stockage	Ech_partieOrga	Spe_code	Spe_dateRec	Spe_lieuRec	Tax_type	Tax_Genre	
5														
6														
7	Extrait Echantillon													
8	Codo	Obligatoir Solvant**	e Disponibilitó	Tune d'extraction	Etat	Brotocolo	Liou do stockoro	Observation	Liconco####	Codo	Disponibilitó	Oupptité	Liou do stockars	
10	Ext code	Ext solvant	Ext dispo	Ext Extraction	Etdl Evt. etat	Ext protocole	Evt stockage	Ext observation	Ext licence	Ech. code	Ech dispo	Ech ate	Ech stockage	4
11	EM_COUC	Ext_solvant	Ext_dispo	Ext_Extraction	CAL_CON	Ext_protocole	Ext_stockube	Ext_observation	Ext_licence	couc	ren_uspo	cen_qee	Ech_stockube	1
12														
13														11
14]		ACETATETYLE	DMSO	11
15				Le fichier CSV d	oit comporter	au minimum les					**Voici la liste	ACETONE	EAU	
16				ch	amps obligato	ires					des solvants	ACETONITRILE	ETHANOL	
17	*La case Al	t doit etre egale	a "IMPORTATION "				L'ordre de	s champs n'est pas i	mportant		present dans L-g	BENZENE	ETHERPET	
10				(nosition	ner sur la nren	nière ligne)					Chimio		METHANOL	
20				(posición)	ner sur la pren	liere lighter						DME	PYRIDINE	
21										-				1
22											Exem	ole de fichier C	sv	
23		A*	В	С	D	E	F	G	н	I. I.	J	K	L	
24	1	IMPORTATION	Ext_code	Ext_solvant	Ext_dispo	Ech_code	Ech_dispo	Ech_qte	Ech_stockage	Ech_partieOrga	Spe_code	Spe_dateRec	Spe_lieuRec	1
25	2		EXT_JOR_01	ETHERETHYL	TRUE	ECH_JOR_2	TRUE	20	sur l'étagère	Feuille	SPE_JOR_01	23/08/2019	Montpellier	-
	< →	Template im	portation Extracto	th 🕂					4				Þ	•

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

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 (<u>Image 46</u>).



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)

***Si vous avez des numéros	Autori	sation	ce sont des champs
d'autorisation à renseigner, vous pouvez les inclure, ils seront liés au	Numéro	Туре	facultatifs. Ils
spécimen présent sur la même ligne.	aut_numero	aut_type	peuvent être mis plusieurs fois.

Picture 47 : Added authorization for the specimen table

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

	A		В		с		D			Е			F		G		н		1			J			
1	IMPORT	ATION	Exp_pa	iys	Tax_ph	ylum	Tax_cla	asse 1	Гах_	Ordr	e Ta	ax_	famille	Тах	type	Тах	_Genre	e Ta	x_Es	pece	Spe_	coo	de		
2			FR		Basidio	myco	Basidio	omyce A	Agar	icale	s A	gar	ricaceae	cha	mpignon	Aga	ricus	an	vens	is	MIC-	001	L		
З			FR		Basidio	myco	Basidio	omyce A	Agar	icale	s A	gar	ricaceae	cha	mpignon	Aga	ricus	ra	dicat	tus	MIC-	002	2		
4			FR		Basidio	myco	Basidio	omyce A	Agar	icale	s Be	olb	oitiaceae	cha	mpignon	Agr	ocybe	pr	aeco	x	MIC-	003	3		
5			FR		Ascom	ycota	Pezizo	mycet F	Peziz	zales	P	yre	enemata	cha	mpignon	Ale	uria	ve	rsic	olor	MIC-	004	1		
6			FR		Basidio	myco	Basidio	omyce A	Agar	icale	s Pl	lut	eaceae	cha	mpignon	Am	anita	ec	hinc	eocep	MIC-	005	5		
	N.								_		D		· ·		-					14	,				
-	N.	0	L	0			P		1	- Cala	n i ava		J Tab ataal		Tala mant		Cala as	,		vv					
5	ре_датеке	cspe_	пеикес	spe_	collectio	spe_	collecte	ECn_CC	bae	ECH	_aisp	01	Ech_stoci	kage	Ecn_part	leoi	ECh_CC	intac	L Ch	_nom					
(01/01/2008	8 Franc	e	Cham	npignon	D. Mi	chelot	MIC-00	01-1	oui		1	spécimer	n da	entier		Aman	d / M	a Ro	land L	upoli				
1	27/10/1986	5 Franc	e	Cham	npignon	D. Mi	chelot	MIC-00	02-1	oui		1	spécimer	n da	entier		Aman	d / M	a Ro	land L	upoli				
(05/06/1986	5 Franc	e	Cham	npignon	D. Mi	chelot	MIC-00	03-1	oui		5	spécimer	n da	entier		Aman	d / M	a Ro	land L	upoli				
1	22/05/1986	5 Franc	e	Cham	pignon	D. Mi	chelot	MIC-00	04-1	oui		5	spécimer	n da	entier		Aman	d/M	a Ro	land L	upoli				
	23/09/1986	5 Franc	e	Cham	npignon	D. Mi	chelot	MIC-00	05-1	oui		5	spécimer	n da	entier		Aman	d/M	a Ro	land L	upoli				
																					•				
	U		W		х			Υ			Z		AA		AB		1	AC		AD			AE		
Ec	h_contact	chi_no	om	Ext	t_code		Ext_so	lvant		Ext_	dispo	E	xt_Extrac	tion	Ext_eta	t	Ext_p	rotoc	ol Ex	(t_sto	ckage	Ext	_obse	rvat	ion
Ar	nand / Ma	Rolan	d Lupol	i Mi	NHN-CX	-0001	METHA	NOL		oui		ag	gitation		en solu	tion	cagitat	ion p	erco	ongéla	teur	2 p	laque	s 96	puit
An	nand / Ma	Rolan	d Lupol	i Mľ	NHN-CX	-0002	METHA	NOL		oui		ag	gitation		en solu	tion	agitat	ion p	erco	ongéla	teur	2 p	laque	s 96	puit
Ar	mand / Ma	Rolan	d Lupol	i Mi	NHN-CX	-0003	METHA	NOL		oui		ag	gitation		en solu	tion	agitat	ion p	erco	ongéla	teur	2 p	laque	s 96	puit
Ar	mand / Ma	Rolan	d Lupol	i Mľ	NHN-CX	-0004	METHA	NOL		oui		ag	gitation		en solu	tion	agitat	ion p	erco	ongéla	teur	2 p	laque	s 96	puit
Ar	mand / Ma	Rolan	d Lupol	i MI	NHN-CX	-0005	METHA	NOL		oui		ag	gitation		en solu	tion	agitat	ion p	erco	ongéla	teur	2 p	laque	s 96	puit

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.

			Moléc	cules de Commu	Chimiothèque nication et Adaptation	ı des Micro-o	rganismes		
Chimiothèque	Ext	raits Échantillor	Condition	spécimen Taxonomie	récolte Autorisation				
Saisie									
Modifications					Modificatio	n d'extraits			
Rechercher	-	10							
	Show	10 V entries						Search:	
Extractothèque	÷	Code 🗘	Solvant 🕴	Type extraction	État 🗍	Disponibilité 🍦	Chimiste ÷	Échantillon	Date d'entrée
• Saisie	0	MNHN-CX-0008	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-008-1	15-05-2023
Modifications Rechercher	0	MNHN-CX-0009	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-009-1	15-05-2023
	0	MNHN-CX-0010	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-010-1	15-05-2023
Administration	0	MNHN-CX-0011	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-011-1	15-05-2023
Chimiothèque Plaques	0	MNHN-CX-0012	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-012-1	15-05-2023
Résultats Bio	0	MNHN-CX-0013	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-013-1	15-05-2023
Importation Exportation	0	MNHN-CX-0014	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-014-1	15-05-2023
Attribution structures	0	MNHN-CX-0015	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-015-1	15-05-2023
Statistiques	0	MNHN-CX-0016	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-016-1	15-05-2023
Extractothèque Importation	0	MNHN-CX-0017	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-017-1	15-05-2023
Exportation	Showin	a 1 to 10 of 751 ent	tries				Previou	c 1 2 3 4	5 76 Next
ParamètresStatistiques		,			Affic	cher	Previou		, o weat

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.

G Google 💿 Partage: Rée	ception 🌐	Intranet MNHN	🐷 Chimiothèque	ChemProducts	···· intranet Collections							
Importation		N-CX-0013	methanol	agitation	en solution dans le methanol	Our	Lupoli Roland	MIC-013-1	15-05-2023			
Exportation	ОМЛН	N-CX-0014	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-014-1	15-05-2023			
Attribution structures	ОМИН	N-CX-0015	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-015-1	15-05-2023			
Statistiques	ОМИН	N-CX-0016	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-016-1	15-05-2023			
Extractothèque Importation	MNHI	N-CX-0017	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-017-1	15-05-2023			
Exportation	Showing 1 to 1	LO of 751 entries					Previous 1	2 3 4 5	. 76 Next			
Paramètres												
Statistiques					Afficher							
Paramètres					Extraits							
Utilisateurs	ID extrait :	MNHN-CX-0017							11.46			
Application	Solvant : m Type extrac	Noditer : Solvant : méthanol Type extraction : agitation										
Compte Compte Déconnexion	Disponibilit Masse disp Protocole : séché, pesé Lieu de sto	Etat : en solution dans le méthanol Disponibilité : Oui Masse disponible (mg) 10 mg Protocole : agitation pendant: 24 à 72H, filtration + évaporation. Repris dans méthanol avec agitation pendant 30 mins et prélèvement du surnageant (un culot sédimenté). Stocké en fiole 30mL à -20°C. 2mL repris séché, pesé et pris dans DMS-d 3 Jong/ml										
	Observatio	ns : 2 plaques 96	puits disponibles pour	le criblage (500 ul à 1	(mg/ml dans le DMSO)							
	Licence : Li	bre										
	Nom du chi Équipe : Bo Date d'entr	imiste : Lupoli Ro do •ée : 15-05-2023	and									
					Purification	IS						
	ID	Purificat	ions		Ref cahier de labo		Fichiers					
	Ajouter											
L-g-Chimio 1.7					i C		Copyright	Laurent ROBIN, CNRS - Univ	ersité d'Orléans 2011			

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.

eque			
	Code echantillon : ATCC 201542-5 Contact : DOI : Stock Non Quantită : 1 g Lieu de stockage : spécimen dans congélateur - 80 Modifier	ID Extraits MNHN-CX-0537	
	ID extrait : MIHN-CX-0537 Solvant : méthanol Type d'extraction : sonication Etat : sec Dispanibilité : Oui Protocole : Extraction par sonication 3 x1 H, le m cupéré en grattant la surface du milieu ris dans x, le milieu ru n'vest par s'exupéré) Lieu de etockage : congélateur 2 - salle chimioth- ge	Etat : Sec Disponibilité : Protocole : Extraction par sonication 3 x1 H, le mycélium est ré cupéré en grattant la surface du milieu riz dans la fiole de roux. (le milieu riz n\'est pas récupéré)	iodifier im est ré im de rou - 1er éta
	Observations 1 2 plaques 96 puits disponibles p (500 µl à 100mg/ml dans le DMSO) Licence I Libre Nom du chimiste : El-Demerdash Amr Equipe I CDNF Purifications ID Purification Ref cabler de labo Ajouter	Lieu de stockage : congélateur 2 - salle chimiothèque - 1er étage Observations : 2 plaques 96 puits disponibles pour le criblage (50 0 ul à 10mg/ml dans le DMSO)	
	Spec	ĥ	Mission de récolte

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.

Chimiothèque Molécules de Communication et Adaptation des Micro-organismes										
Chimiothèque Saisie	Extra	its Échantillon	Condition spécir	nen Taxonomie récol	Recharche d'orter	ite				
Rechercher	Show 10 v entries Search:									
Extractothèque	÷	Code	Solvant 🕴	Type extraction	État 🗘	Disponibilité 🕴	Chimiste $\frac{1}{2}$	Échantillon 🗧		
Saisie	0	MNHN-CX-0008	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-008-1		
 Modifications Rechercher 	0	MNHN-CX-0009	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-009-1		
	0	MNHN-CX-0010	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-010-1		
Administration	0	MNHN-CX-0011	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-011-1		
Chimiothèque Plaques	0	MNHN-CX-0012	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-012-1		
Résultats Bio	0	MNHN-CX-0013	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-013-1		
Exportation	0	MNHN-CX-0014	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-014-1		
Attribution structures	0	MNHN-CX-0015	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-015-1		
Statistiques	0	MNHN-CX-0016	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-016-1		
Extractotheque Importation	0	MNHN-CX-0017	méthanol	agitation	en solution dans le méthanol	Oui	Lupoli Roland	MIC-017-1		
 Exportation Paramètres 	Showing	1 to 10 of 751 entries	s				Previous 1 2 3	4 5 76 Next		
Statistiques					Rechercher					



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.

Code specimen : AN312R		
Date de recolte : 2013-01-01 Lieu de recolte : roscoff (France) Position GPS :		
Observations :		
Collection : Mycologie UMR 7245 Contact : S. Prado Collecteur : M. Vallet Voir les fichiers		
	Echantillon	
Code echantillon : AN312R-1	Code echantillon : AN312R-2	
Contact :	Contact :	
DOI :	DOI :	
Stock : Non Quantté : 1 g Lieu de stockage : spécimen dans congélateur -80°C - souchier - service mycologie UMR 7545	Stock : Non Quantité : 1 g Lieu de stockage : spécimen dans congélateur -80°C - souchier - service mycologie UMR 7545	
L	L	
Minim de cécules		Touronais
Mission de recoite		laxonomie
ID Mission de récolte : 49		ID taxonomie : 458
Nom : MNHN-roscoff-Algue		Phylum :
Contact : S. PRADO		Ordre :
Pays : FRANCE Collaboration : Non		Famille : Genre : Penicillium

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.

	Chimiothèque Institut de Chimie Organique et Analytique	icoa
Clondelleque Sainie Modifications Hostinata Bio Recerctore Sainie Sainie Sainie Katheritations Rechercher Compte Compte Compte Compte Compte	Inter addresse.couriel i: @ bui i: @ bui i: Inner: Inner: Inner: Inner: Inner: Inner: Saidr le nouveau mot de passe : Confirmez le nouveau mot de passe : Hot de passe actuel : Soumettre	Option visible uniquement pour les niveaux : administrateur, chef et responsable.
L-g-Chimio 1.7	ii C	Copyright Laurent ROBIN, CNRS - Université d'Orléans 2011

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





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.



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.





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.





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https://cn-intra.enscm.fr/chidept.html

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Crossings



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.

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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.

Note on configuration : 3R, 5R 25% 3R, 5S 30% 3S, 5S 15%

> Note on configuration : 2S, 4S or 2R, 4R

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.

5



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.

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