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Présentation du projet Madbot au All-Hands IFB/ELIXIR-FR 2024

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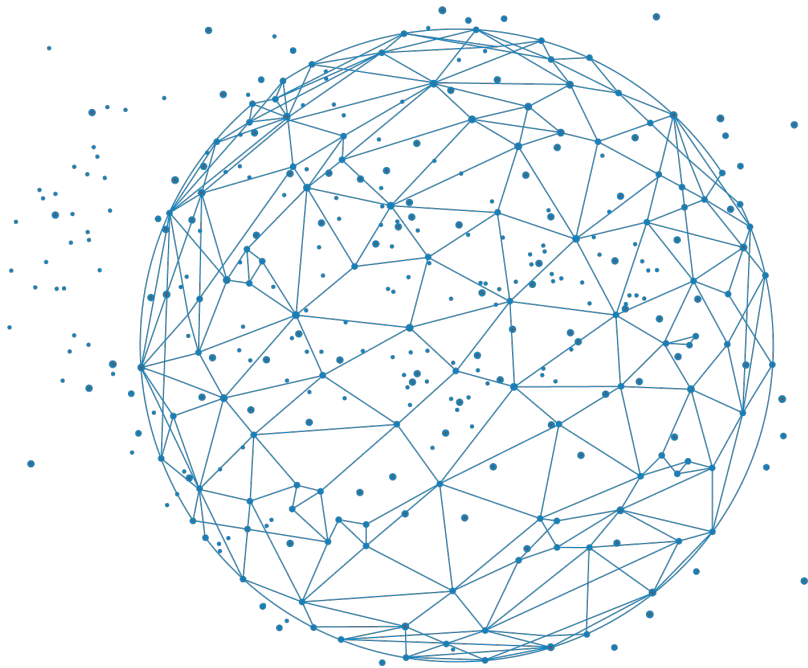
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MADBOT

Metadata And Data Brokering Online Tool

Laurent Bouri, Imane Messak, Baptiste Rousseau



- Présenter l'équipe
- C'est quoi madbot ?
 - notre objectif
 - Pourquoi utiliser madbot ?
 - ✓ Une structure ISA
 - ✓ Les connecteurs
 - ✓ Les datalinks
 - ✓ les data
 - ✓ Les métadonnées
 - La soumission de données
- notre MVP (Minimum Viable Product)
 - Pourquoi un MVP? (ena/zenodo soumission de data)
- Notre code
 - ✓ pipeline (ci gitlab)
 - ✓ Architecture

L'équipe MADBOT



IFB
INSTITUT FRANÇAIS DE BIOINFORMATIQUE

Julien Seiler
IR CNRS
(Strasbourg)

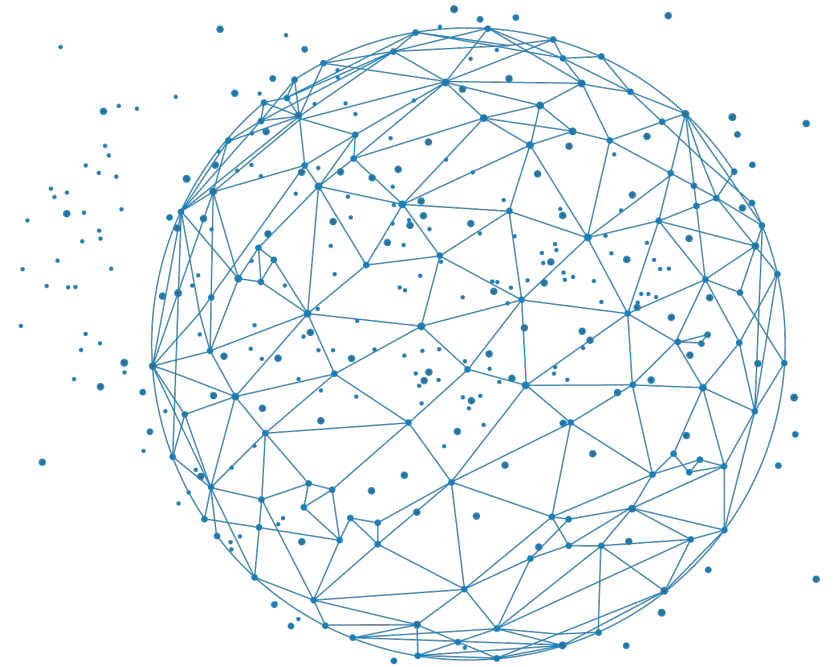
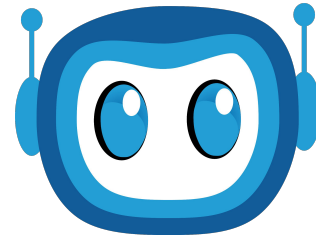
Thomas Denecker
IR CNRS
(Paris)

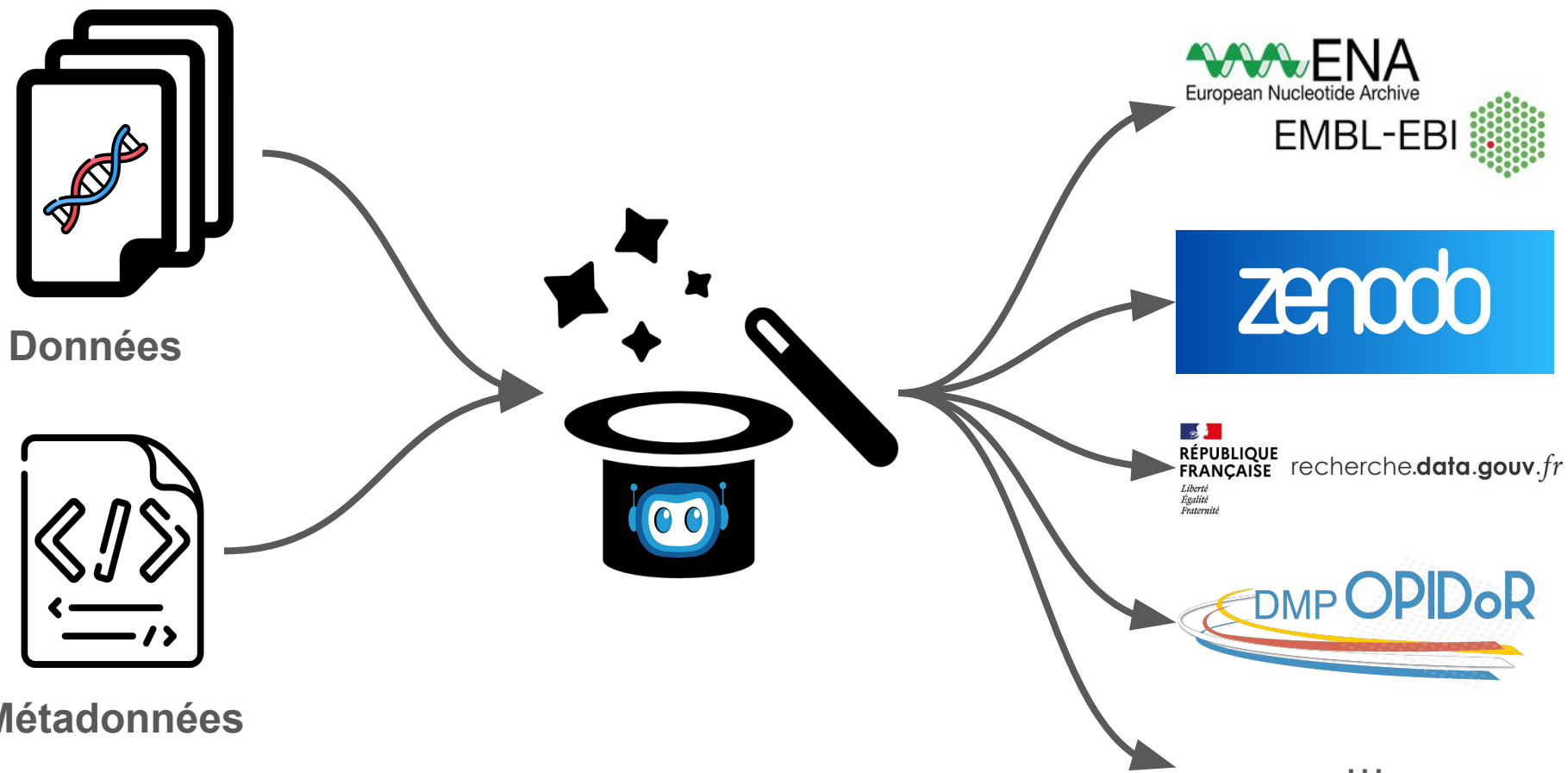
Laurent Bouri
IR CNRS
(Strasbourg)

Baptiste Rousseau
IR CNRS
(Paris)

Imane Messak
IR CNRS
(Paris)

C'est quoi MADBOT?

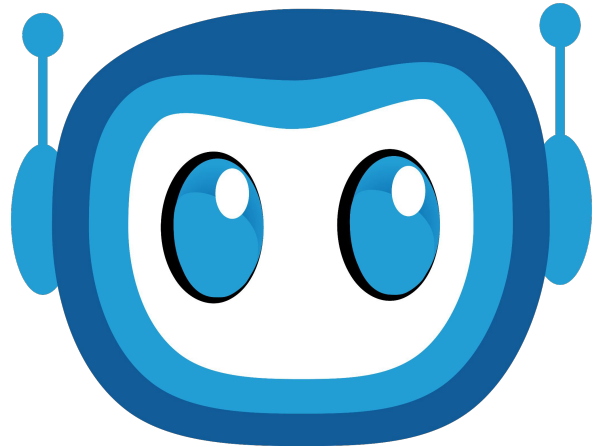






MADBOT (Metadata And Data Brokering Online Tool) est une application web qui fournit **un tableau de bord pour la gestion des données et des métadonnées de recherche.**

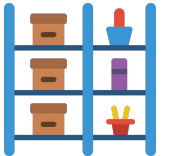


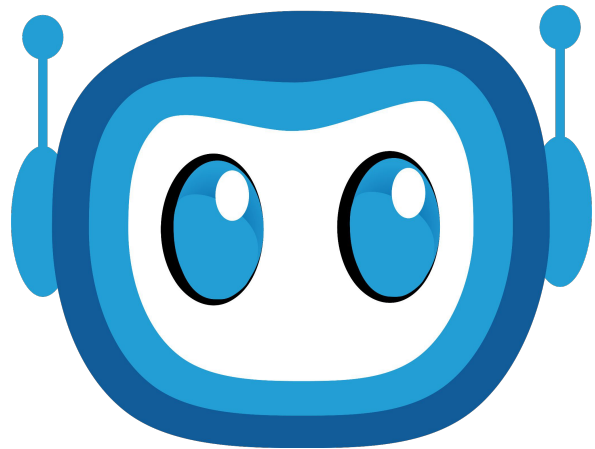


MADBOT (Metadata And Data Brokering Online Tool) est une application web qui fournit **un tableau de bord pour la gestion des données et des métadonnées de recherche.**



L'application permet d'**agrég**er les **métadonnées** autour de projets scientifiques et d'**identifier précisément où sont stockées les données** au travers de nombreux connecteurs.

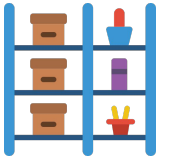




MADBOT (Metadata And Data Brokering Online Tool) est une application web qui fournit **un tableau de bord pour la gestion des données et des métadonnées de recherche.**



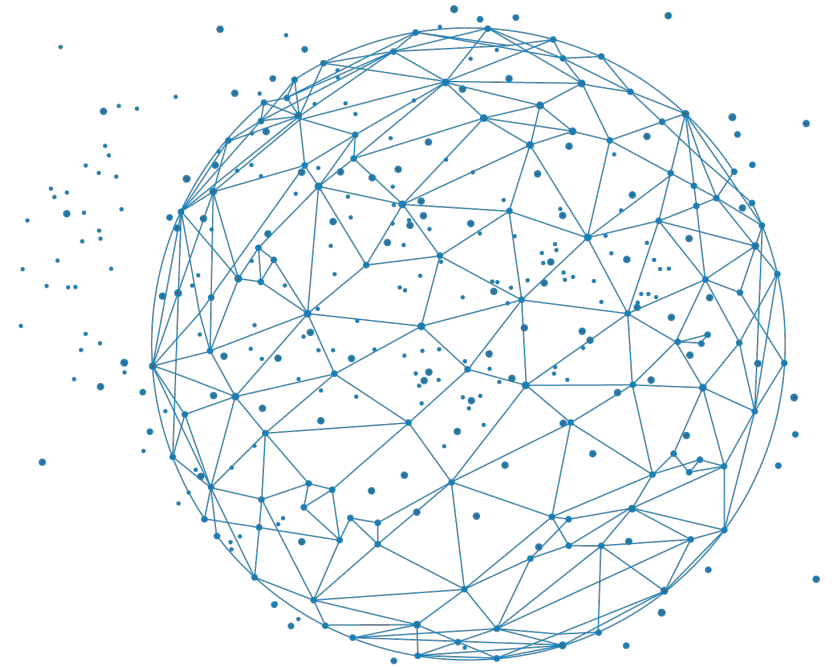
L'application permet d'**agréger les métadonnées** autour de projets scientifiques et d'**identifier précisément où sont stockées les données** au travers de nombreux connecteurs.



Elle accompagne également les chercheurs pour la **publication des données et des métadonnées** vers un grand nombre d'entrepôts généraliste (RGD, Zenodo, etc.) et thématique (ENA, GEO, etc.)



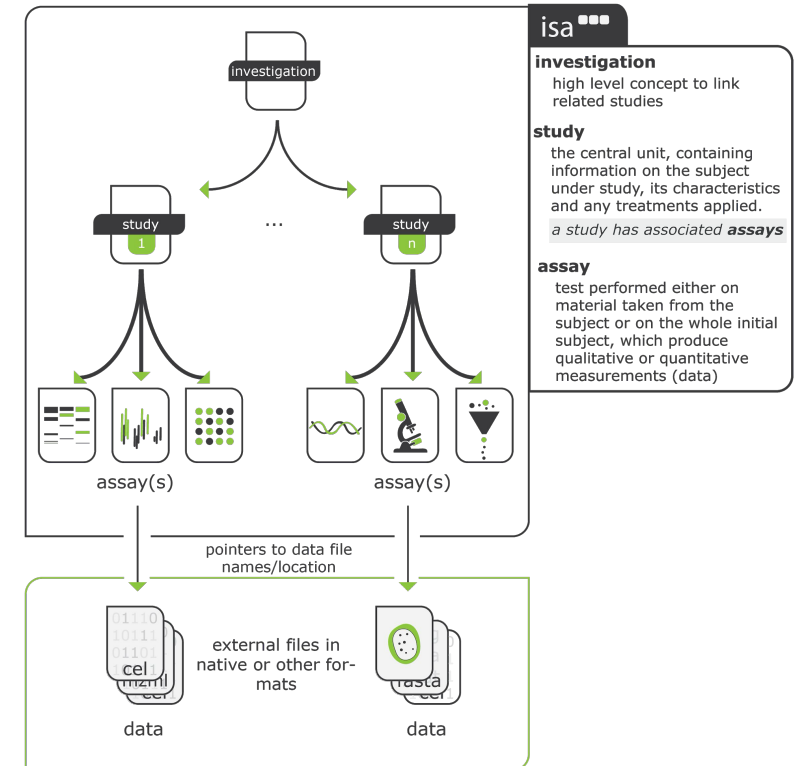
Comment ça fonctionne ?





Au sein de **MADBOT**, chaque projet de recherche est décrit sous la forme d'un ensemble de **Nodes** qui peuvent être des **investigations**, des **études (study)** et des **expériences (assay)**, cela sous la forme d'un arbre hiérarchique (modèle ISA). Ces ensembles de **Nodes** sont regroupés dans des workspaces.

- **Investigation** : le contexte du projet
- **Study** : une expérimentation en un seul lieu
- **Assay** : une mesure spécifique qui cible un trait avec une méthode et une échelle.

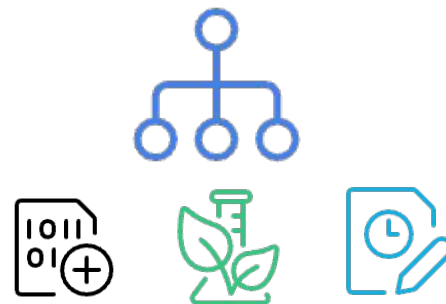


Sources : <https://isa-tools.org> et <https://isa-specs.readthedocs.io/en/latest/isamodel.html>



Mais nous ne nous limitons pas qu'au modèle ISA et nous prévoyons de mettre en place de nouvelles collections de type de *Nodes*.

Chaque élément de cet arbre peut être associés à des données, des échantillons biologiques et des métadonnées.





MADBOT

Parameters

Welcome to Madbot

Madbot allows you to identify and track the data and metadata associated with the different stages of your research projects.

To get started, you need to create at least one workspace.

A workspace lets you organize your work as you wish, for yourself, your team or an entire organization.

A workspace name is required to start.

START

Imane Messak





MADBOT

Parameters

Welcome to Madbot

Madbot allows you to identify and track the data and metadata associated with the different stages of your research projects.

To get started, you need to create at least one workspace.

A workspace lets you organize your work as you wish, for yourself, your team or an entire organization.

Workspace name

my team workspace

START

Imane Messak



MADBOT

MY TEAM WORKSPACE

- Dashboard
- Inbox
- Parameters
- Submissions
- New investigation

Dashboard



No datalinks found

It's time to link some data!

Create your first node and go to the Datalinks tab to identify where your data are located. ✎

NEW INVESTIGATION

Imane Messak



Création d'un Node Investigation



MADBOT ☰

MY TEAM WORKSPACE ▼

- Dashboard
- Inbox
- Parameters
- Submissions
- New investigation
- ▼ **Untitled**

Everything saved ...

Untitled

investigation

Choose how to create this investigation...

- EMPTY INVESTIGATION
- DEMO INVESTIGATION

Imane Messak → ?



MADBOT

MY TEAM WORKSPACE

- Dashboard
- Inbox
- Parameters
- Submissions
- New investigation

- Growth control of the eukaryot...
 - A time course analysis of tran...
 - Study of the impact of change...

Growth control of the eukar... Everything saved

Growth control of the eukaryote cell: a systems biology study in yeast

investigation

Background Cell growth underlies many key cellular and developmental processes, yet a limited number of studies have been carried out on cell-growth regulation. Comprehensive studies at the transcriptional, proteomic and metabolic levels under defined controlled conditions are currently lacking. Results Metabolic control analysis is being exploited in a systems biology study of the eukaryotic cell. Using chemostat culture, we have measured the impact of changes in flux (growth rate) on the transcriptome, proteome, endometabolome and exometabolome of the yeast *Saccharomyces cerevisiae*. Each functional genomic level shows clear growth-rate-associated trends and discriminates between carbon-sufficient and carbon-limited conditions. Genes consistently and significantly upregulated with increasing growth rate are frequently essential and encode evolutionarily conserved proteins of known function that participate in many protein-protein interactions. In contrast, more unknown, and fewer essential, genes are downregulated with increasing growth rate; their protein products rarely interact with one another. A large proportion of yeast genes under positive growth-rate control share orthologs with other eukaryotes, including humans. Significantly, transcription of genes encoding components of the TOR complex (a major controller of eukaryotic cell growth) is not subject to growth-rate regulation. Moreover, integrative studies reveal the extent and importance of post-transcriptional control, patterns of control of metabolic fluxes at the level of enzyme synthesis, and the relevance of specific enzymatic reactions in the control of metabolic fluxes during cell growth. Conclusion This work constitutes a first comprehensive systems biology study on growth-rate control in the eukaryotic cell. The results have direct implications for advanced studies on cell growth, in vivo regulation of metabolic fluxes for comprehensive metabolic engineering, and for the design of genome-scale systems biology models of the eukaryotic cell.

DATALINKS 0 SAMPLES 0 METADATA 0 STUDY 2

NEW DATALINK

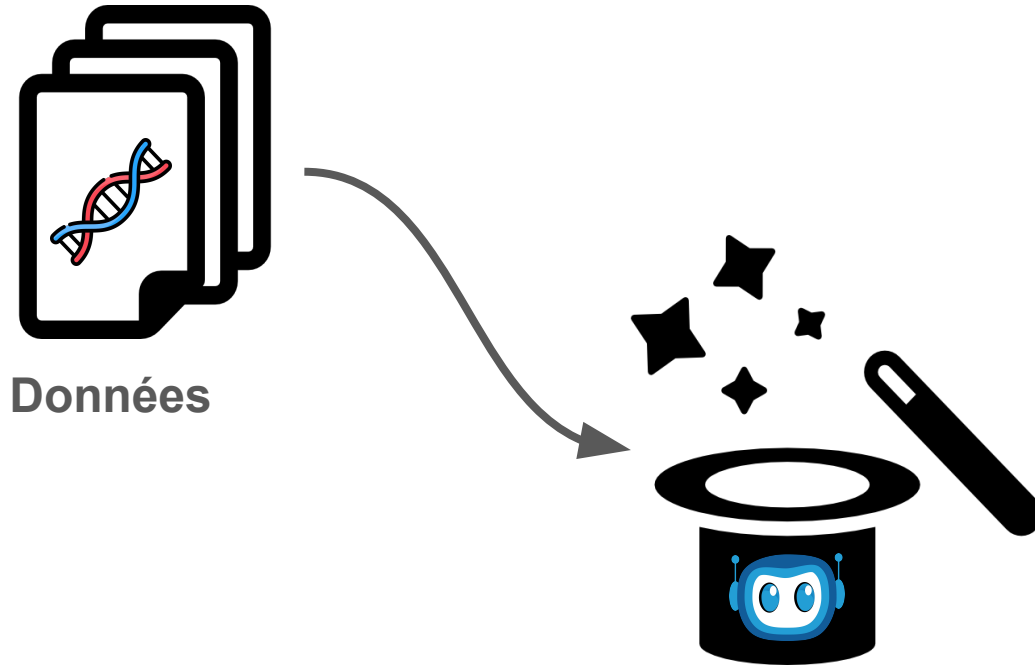
Name	Connections	Data access
------	-------------	-------------

No data available

Items per page: 10 0-0 of 0 < >

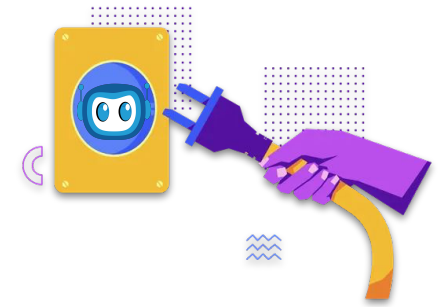
Imane Messak





Les connecteurs sont des modules Python permettant d'accéder aux données d'**outils de gestion de données**, tels que Galaxy, via leurs API.

Conçus de manière **modulaire**, les connecteurs de MADBOT permettent à chacun de **contribuer en développant de nouveaux connecteurs** adaptés à ses besoins.



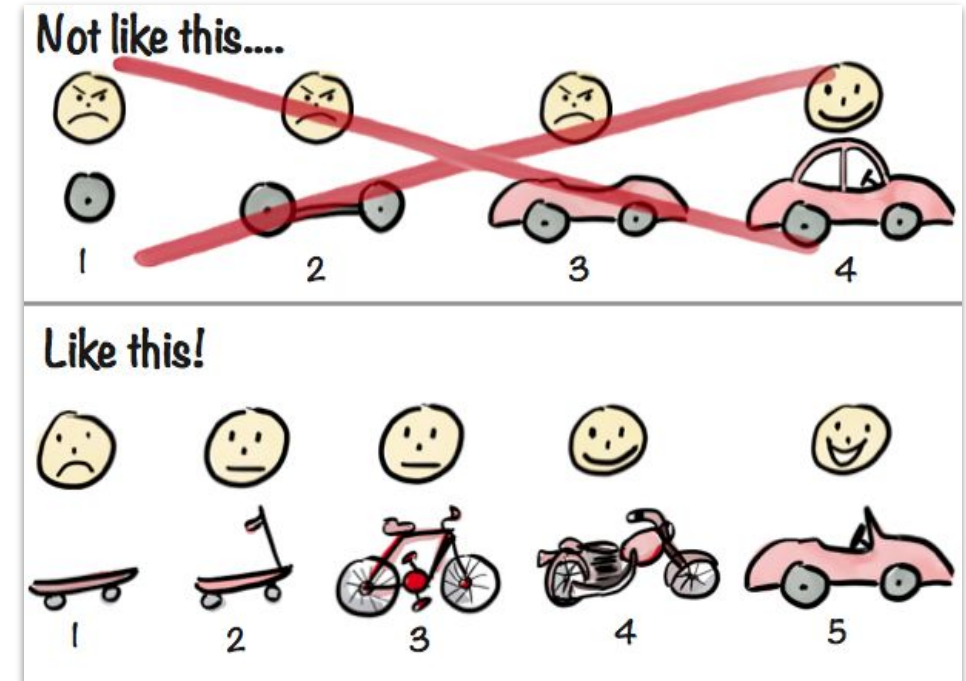


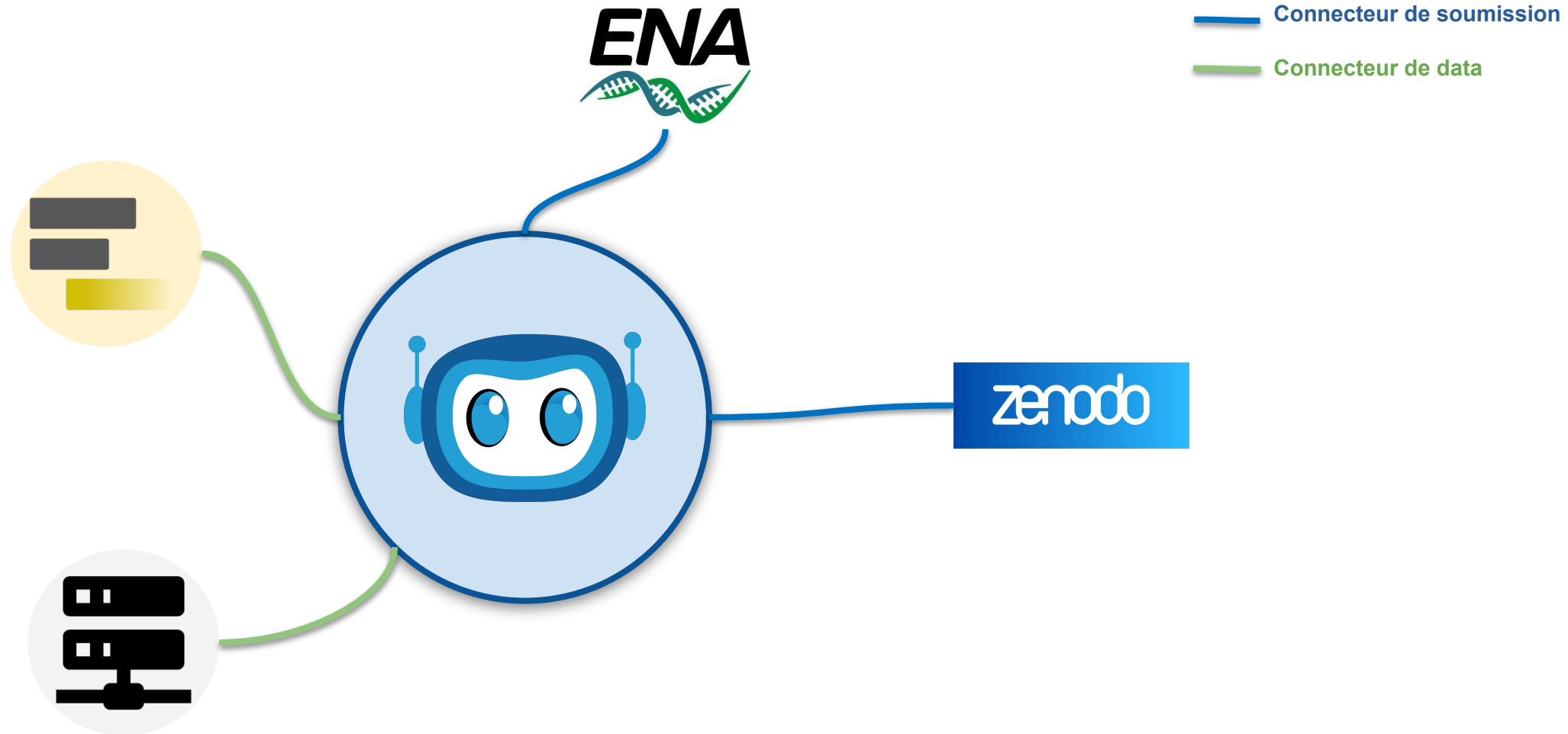
Nous souhaitons produire le plus rapidement possible une application fonctionnelle.

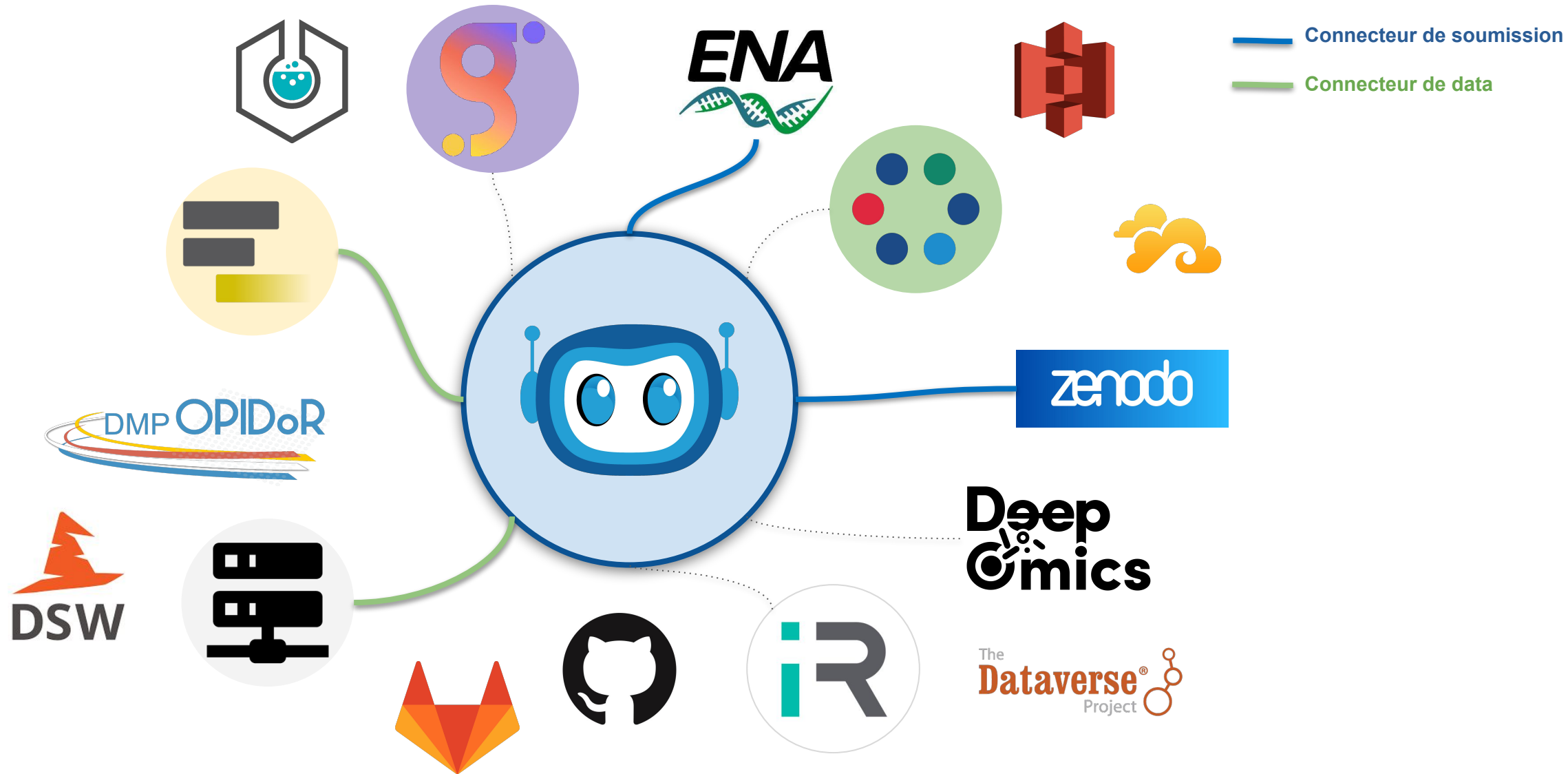
Objectifs principaux

- Démontrer que nous pouvons associer à un arbre ISA des données localisées sur différents systèmes de stockage (Galaxy et SSHFS)
- Démontrer que nous pouvons renseigner des métadonnées pour un arbre ISA et ses données
- Démontrer que nous pouvons publier ces données sur des entrepôts de références thématiques (ENA) et non thématiques (Zenodo).

L'application MADBOT capable de réaliser ces objectifs est notre **Minimal Viable Product (MVP)**.

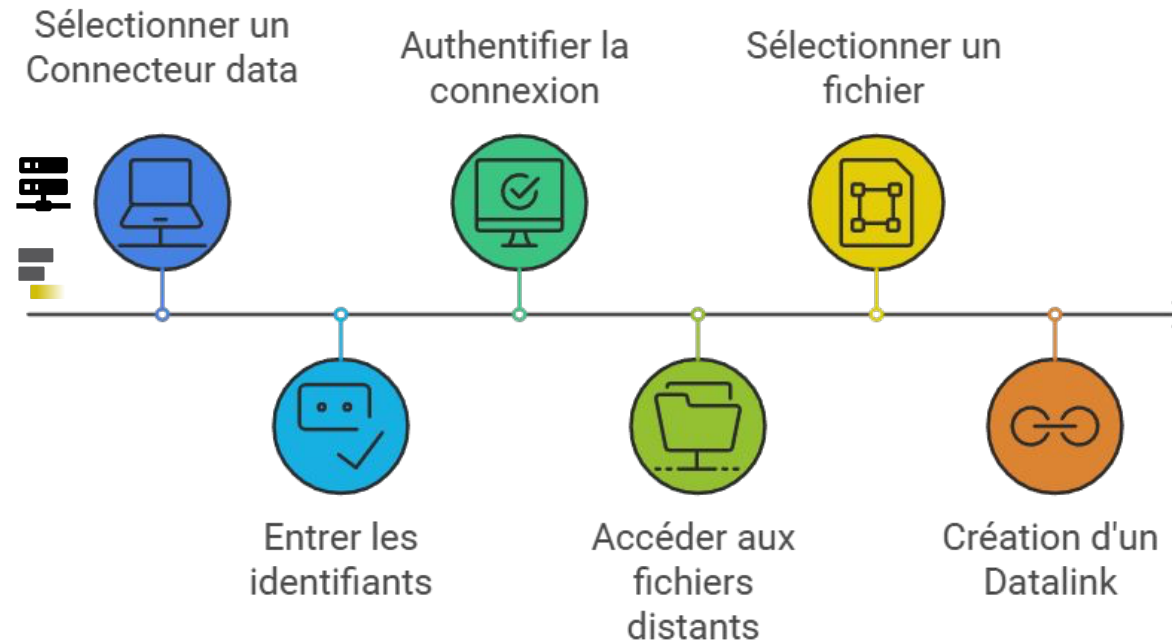








Un datalink est un **lien** entre **une donnée accessible à distance** via un connecteur et un **Node**.
Ainsi, **aucun fichier n'est stocké en local**.





MADBOT

MY TEAM WORKSPACE

- Dashboard
- Inbox
- Parameters
- Submissions
- New investigation

▼ **Growth control of the eukaryot...**

- > A time course analysis of tran...
- > Study of the impact of change...

Growth control of the eukar... Everything saved

Growth control of the eukaryote cell: a systems biology study in yeast

investigation

Background Cell growth underlies many key cellular and developmental processes, yet a limited number of studies have been carried out on cell-growth regulation. Comprehensive studies at the transcriptional, proteomic and metabolic levels under defined controlled conditions are currently lacking. Results Metabolic control analysis is being exploited in a systems biology study of the eukaryotic cell. Using chemostat culture, we have measured the impact of changes in flux (growth rate) on the transcriptome, proteome, endometabolome and exometabolome of the yeast *Saccharomyces cerevisiae*. Each functional genomic level shows clear growth-rate-associated trends and discriminates between carbon-sufficient and carbon-limited conditions. Genes consistently and significantly upregulated with increasing growth rate are frequently essential and encode evolutionarily conserved proteins of known function that participate in many protein-protein interactions. In contrast, more unknown, and fewer essential, genes are downregulated with increasing growth rate; their protein products rarely interact with one another. A large proportion of yeast genes under positive growth-rate control share orthologs with other eukaryotes, including humans. Significantly, transcription of genes encoding components of the TOR complex (a major controller of eukaryotic cell growth) is not subject to growth-rate regulation. Moreover, integrative studies reveal the extent and importance of post-transcriptional control, patterns of control of metabolic fluxes at the level of enzyme synthesis, and the relevance of specific enzymatic reactions in the control of metabolic fluxes during cell growth. Conclusion This work constitutes a first comprehensive systems biology study on growth-rate control in the eukaryotic cell. The results have direct implications for advanced studies on cell growth, in vivo regulation of metabolic fluxes for comprehensive metabolic engineering, and for the design of genome-scale systems biology models of the eukaryotic cell.

DATALINKS 0 SAMPLES 0 METADATA 0 STUDY 2

NEW DATALINK

Name	Connections	Data access
No data available		

Items per page: 10 0-0 of 0 < < > >

Imane Messak



MADBOT Growth control of the eukar... Everything saved

MY TEAM WORKSPACE

- Dashboard
- Inbox
- Parameters
- Submissions
- New investigation

Growth control of the eukaryote cell: a systems biology study in yeast

Add a datalink

1 Choose a connector — 2 Connect — 3 Select a data

Choose an existing connection

No more items

Create a new connection from a connector

- Galaxy
- SSHFS

or

NEW DATALINK

Imane Messak



The screenshot shows the MADBOT web interface. The main header displays 'MADBOT' and the current workspace 'MY TEAM WORKSPACE'. The page title is 'Growth control of the eukaryote cell: a systems biology study in yeast'. A sidebar on the left contains navigation options: Dashboard, Inbox, Parameters, Submissions, and New investigation. The main content area is partially obscured by a modal dialog box titled 'Add a datalink'. The dialog has a progress bar with three steps: 'Choose a connector' (completed), 'Connect' (current step), and 'Select a data'. The 'Connect' step contains a form for connecting to Galaxy, with sections for 'Shared parameters' and 'Private parameters'. The 'Shared parameters' section includes a dropdown for 'Galaxy Instances' and a text field for 'Url Galaxy' with a red asterisk and the note 'is a required property'. The 'Private parameters' section includes a text field for 'Login*' and a password field for 'Password*', both with red asterisks and the note 'is a required property'. The dialog also features a 'BACK' button and a 'CONNECT' button. In the background, a 'NEW DATALINK' button is visible on the right side of the page.



The screenshot shows the MADBOT web interface. At the top, the title is "Growth control of the eukaryote cell: a systems biology study in yeast". A modal dialog box titled "Add a datalink" is open, showing a progress bar with three steps: "Choose a connector" (checked), "Connect" (current step), and "Select a data".

Complete the form below to connect to Galaxy

Shared parameters

- Galaxy Instances: [Dropdown menu]
- Uri Galaxy: Galaxy France (The Galaxy platforms.)

Private parameters

- Login*: imane.messak@france-bioinformatique.fr (The username or email address used for authentication.)
- Password*: [Masked] (The user's password, which must be kept confidential.)

Buttons: BACK, CONNECT

Background text (partially visible): "on cell-growth regulation. results Metabolic control changes in flux (growth rate) on vel shows clear growth-rate- lated with increasing growth actions. In contrast, more er. A large proportion of yeast coding components of the e extent and importance of tic reactions in the control of in the eukaryotic cell. The ngineering, and for the design"



MADBOT Growth control of the eukar... Everything saved

MY TEAM WORKSPACE

- Dashboard
- Inbox
- Parameters
- Submissions
- New investigation

Growth control of the eukaryote cell: a systems biology study in yeast

Add a datalink

1 Choose a connector 2 Connect 3 Select a data

All histories/

- NC_0445512.2 reference sequence
- Assembly
- Imaging
- COVID ressources
- assembly and chipseq
- fasta NC_045512
- covid test data

Galaxy
Galaxy France

NEW DATALINK

BACK CREATE DATALINK

Imane Messak



MADBOT Growth control of the eukar... Everything saved

MY TEAM WORKSPACE

Dashboard
Inbox
Parameters
Submissions
New investigation

Growth control of the eukaryote cell: a systems biology study in yeast

Add a datalink

1 Choose a connector 2 Connect 3 Select a data

All histories/

- NC_0445512.2 reference sequence
- Assembly**
- Imaging
- COVID ressources
- assembly and chipseq
- fasta NC_045512
- covid test data

Galaxy
Galaxy France

Assembly
Galaxy History

BACK CREATE DATALINK

NEW DATALINK

Imane Messak



MADBOT

MY TEAM WORKSPACE

- Dashboard
- Inbox
- Parameters
- Submissions
- New investigation

▼ **Growth control of the eukaryot...**

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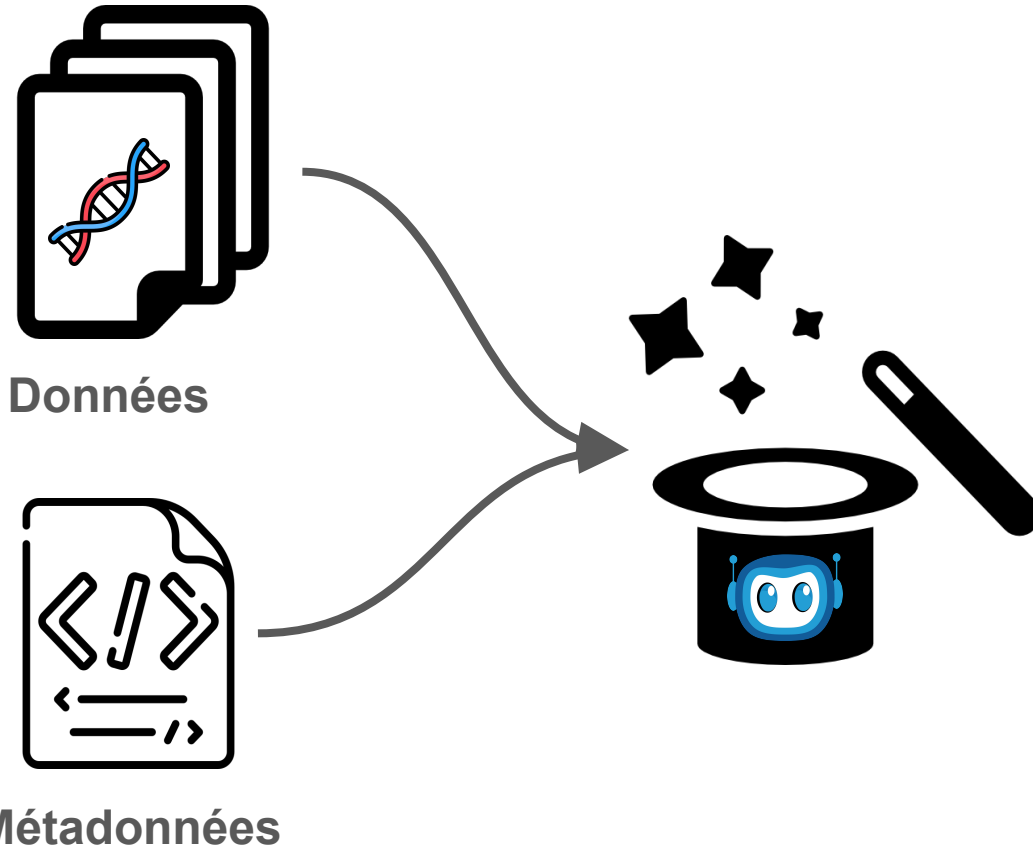
DATALINKS 0 SAMPLES 0 METADATA 0 STUDY 2

NEW DATALINK

Name	Connections	Data access
Assembly 0.00 octets	Galaxy France	Accessible

Items per page: 10 1-1 of 1

Imane Messak





Comment décrire les données ?

- Avec des métadonnées



Comment décrire les données ?

- Avec des métadonnées



Les données



Comment décrire les données ?

- Avec des métadonnées



Les données



Comment décrire les données ?

- Avec des métadonnées



Les données



Les métadonnées



Comment décrire les données au mieux ?

- Avec un standard

In essence, a standard is an **agreed way of doing something**.

A standard provides the **requirements, specifications, guidelines** or **characteristics** that can be used for the **description, interoperability, citation, sharing, publication, or preservation** of all kinds of **digital objects** such as data, code, algorithms, workflows, software, or papers.

source: <https://fairsharing.org/educational/>

Quels sont les standards à notre disposition ?

- Pour l'**ENA**, les checklists

Une checklist définit les métadonnées minimales et optionnelles attendues pour décrire un échantillon biologique

Elles sont basées sur les recommandations du Genomic Standards Consortium (GSC)

La checklist la plus appropriée dépend du type d'échantillon :

<https://www.ebi.ac.uk/ena/browser/checklists>

- Et pour les autres ?

Checklist: ERC000020 ?

GSC MixS plant associated

Genomic Standards Consortium package extension for reporting of measurements and observations obtained from the environment where the sample was obtained. By choosing the environmental package, a selection of fields can be made from a relevant subsets of the GSC terms.

Checklist Fields ?

Filter fields...

Filter by type:

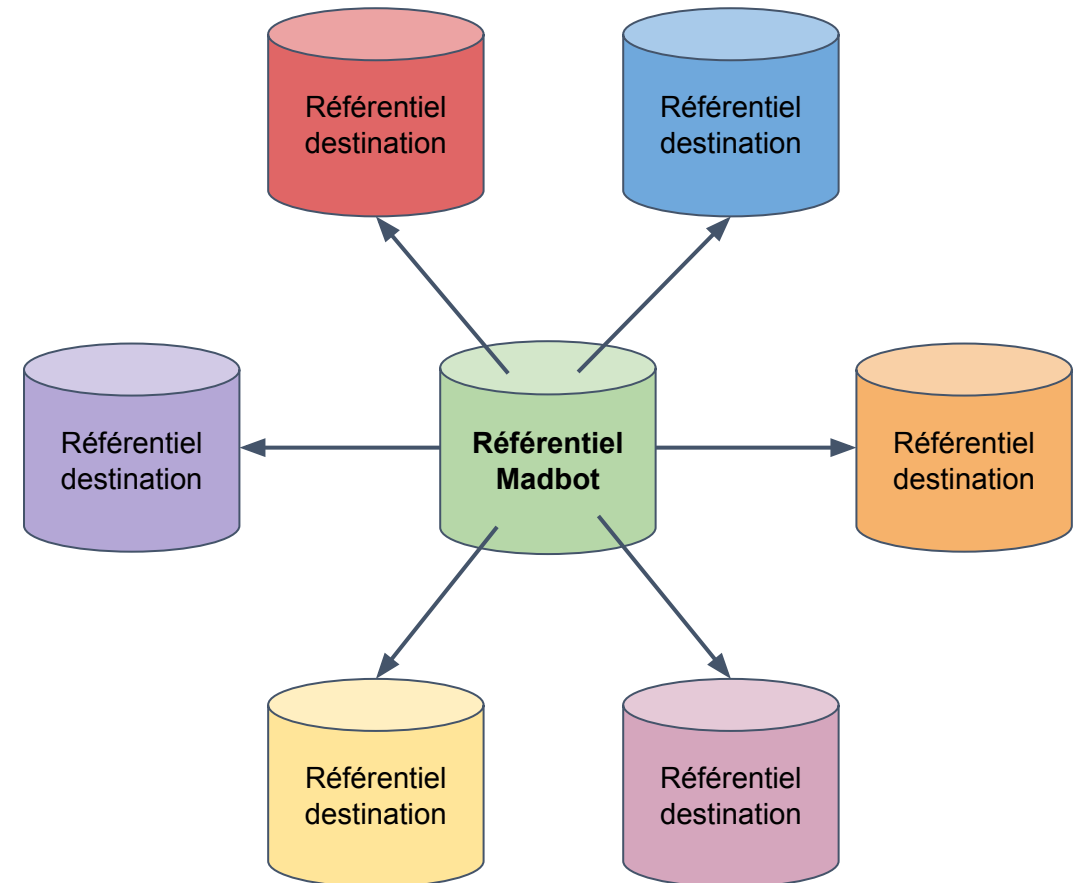
- non-sample terms
- Collection event information
- sample collection
- host disorder
- host description
- local environment conditions
- concentration measurement
- host details
- organism characteristics
- local environment conditions imposed

Field Name	Field Format	(Field Restriction)	Requirement	(Units)
project name	free text		mandatory	
experimental factor	free text		optional	
ploidy	free text		optional	
number of replicons	restricted text	regular expression	optional	
extrachromosomal elements	restricted text	regular expression	optional	
estimated size	restricted text	regular expression	optional	
reference for biomaterial	free text		optional	
annotation source	free text		optional	
sample volume or weight for DNA extraction	restricted text	regular expression	optional	options
nucleic acid extraction	free text		optional	
nucleic acid amplification	free text		optional	
library size	restricted text	regular expression	optional	
library reads sequenced	restricted text	regular expression	optional	



Compte tenu de la grande diversité des standards de métadonnées et de leur faible interopérabilité, nous avons fait le choix de créer un référentiel de métadonnées propres à MADBOT.

Ce référentiel jouera le rôle de langage universel pour saisir l'ensemble des métadonnées au sein des arborescences de *Node*, *Sample* et *Data* de MADBOT.





Des métadonnées peuvent être associées aux *Nodes*, *Samples*, *Data* et associations entre *Data*

Des métadonnées peuvent être associées aux *Nodes*, *Samples*, *Data* et associations entre *Data*

En cherchant un champ de métadonnée du référentiel MADBOT

The screenshot displays the MADBOT web interface. On the left, a sidebar shows navigation options: 'Submissions', 'New investigation', and a selected investigation titled 'Growth control of the eukaryot...' with a sub-entry 'Study of the impact of change...'. The main content area shows a text snippet from a scientific paper. A modal window titled 'Add metadata' is open, featuring a search bar with 'taxon' entered. Below the search bar, it states 'Metadata fields found: 6'. Three categories of metadata fields are listed, each with a 'Mapped with' button and a trash icon:

- Host specie taxon**: Specie rank *taxon* of the host to the organism from which sample was obtained. Mapped with: host scientific name, host scientific name.
- Sample specie taxon**: Specie rank *taxon* of the sample based on the NCBI taxonomy database. Mapped with: subjects, tax_id, scientific_name.
- Sample sub-species taxon**: Name of sub-species of organism from which sample was obtained. Mapped with: sub-species scientific name.

At the bottom of the modal, there is a 'Selected metadata fields' section and an 'ADD TO METADATA' button. The background interface includes a 'SAVE' button, a 'NEW METADATA' dropdown menu, and a pagination indicator '1-3 of 3'.

Des métadonnées peuvent être associées aux *Nodes*, *Samples*, *Data* et associations entre *Data*

En cherchant à partir d'un référentiel externe

The screenshot displays the MADBOT interface with a modal window for adding metadata. The background shows a submission page with a text description of a study on yeast metabolic control. The modal window is titled "Add metadata by mapping" and is divided into two main sections:

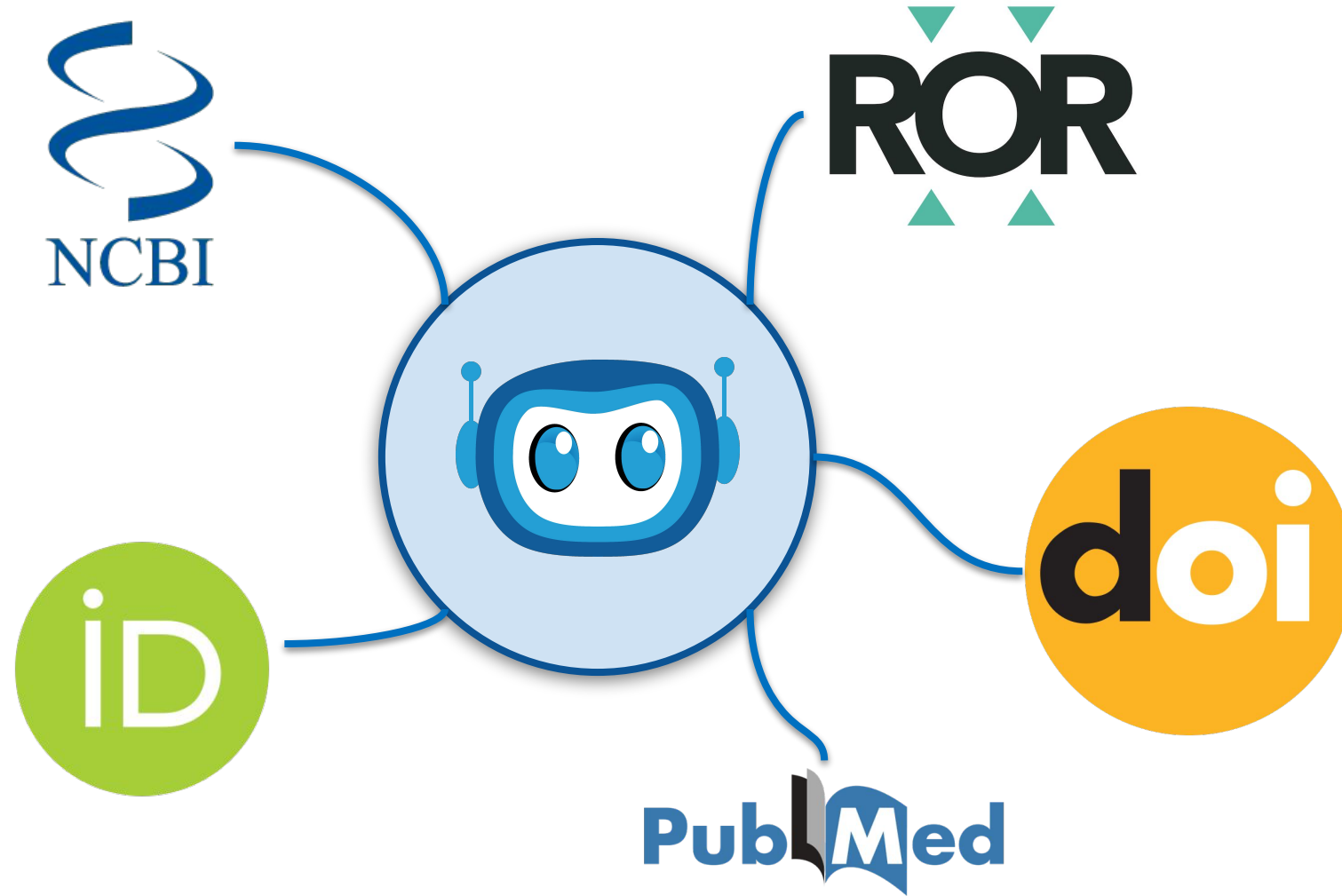
- Left Panel:** A tree view of external references. The "Sample" category is expanded, showing "ERC000011 - Default sample checklist" as the selected item.
- Right Panel:** A list of 22 metadata fields being mapped to sample attributes. The fields include: cell_line, cell_type, collection date, cultivar, dev_stage, geographic location (two instances), lat/lon, host scientific name, environment, germline, and isolate. Each field has a corresponding input field and a star icon for marking it as required.

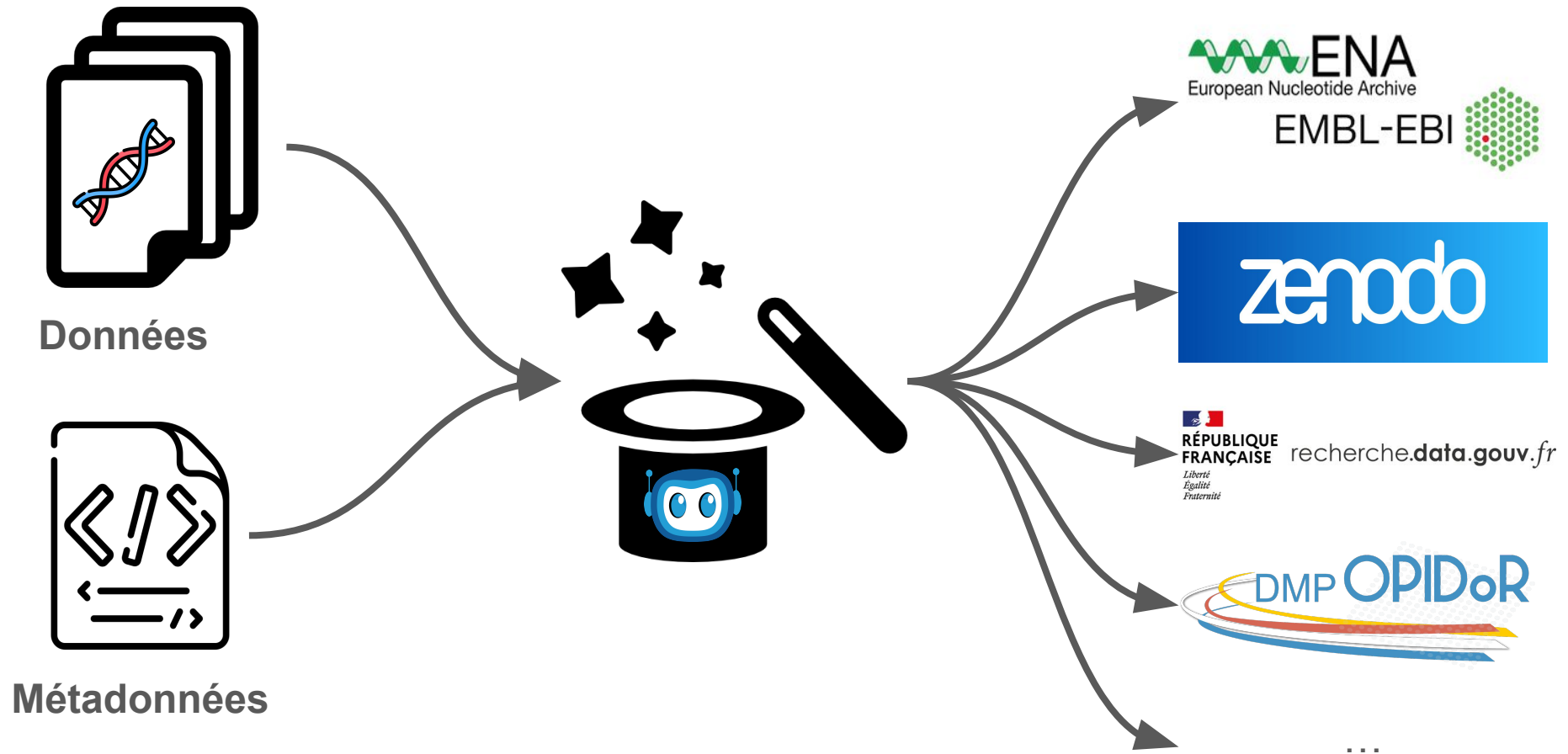
At the bottom of the modal, there is a "Selected metadata fields" box and an "ADD TO METADATA" button.

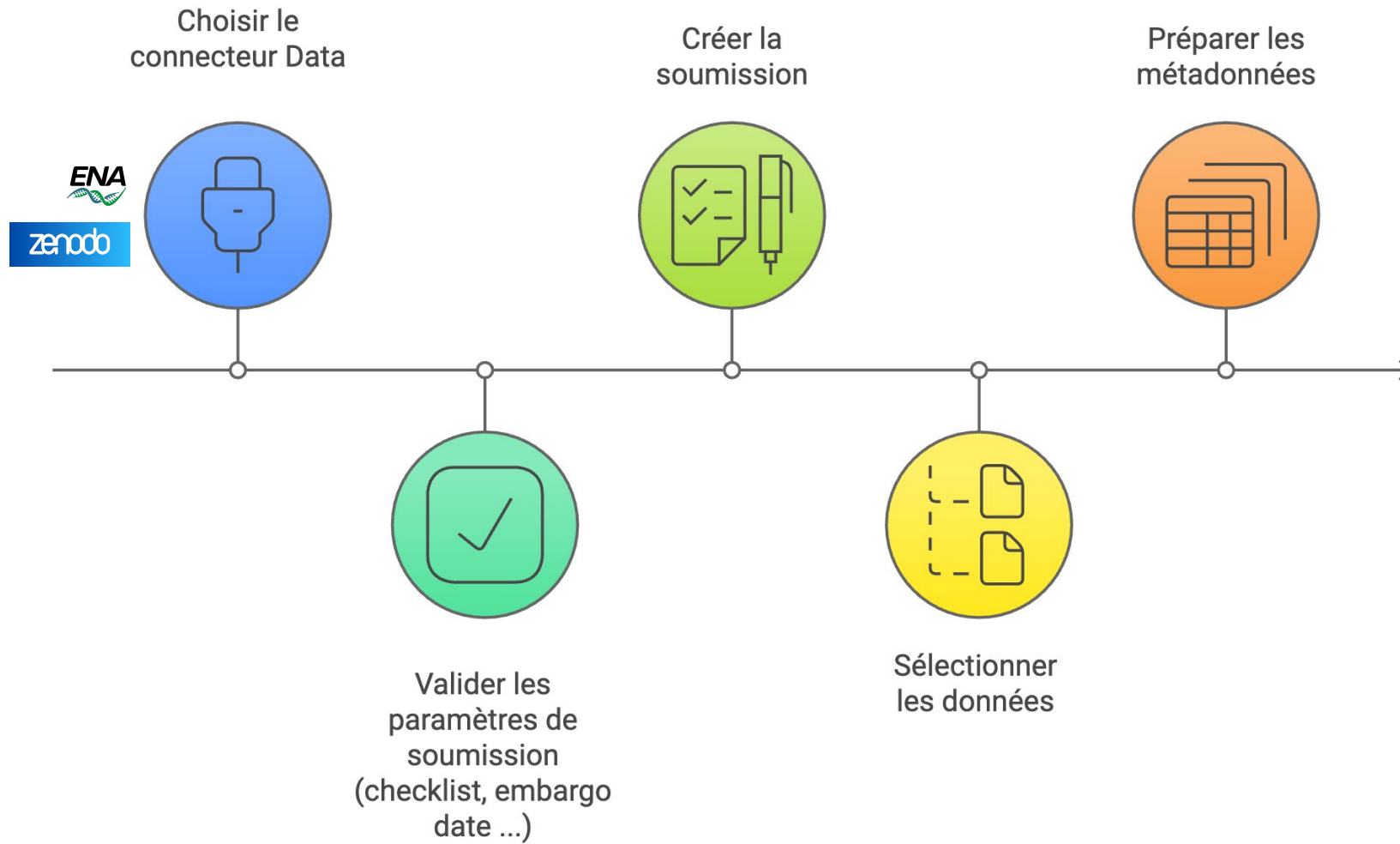


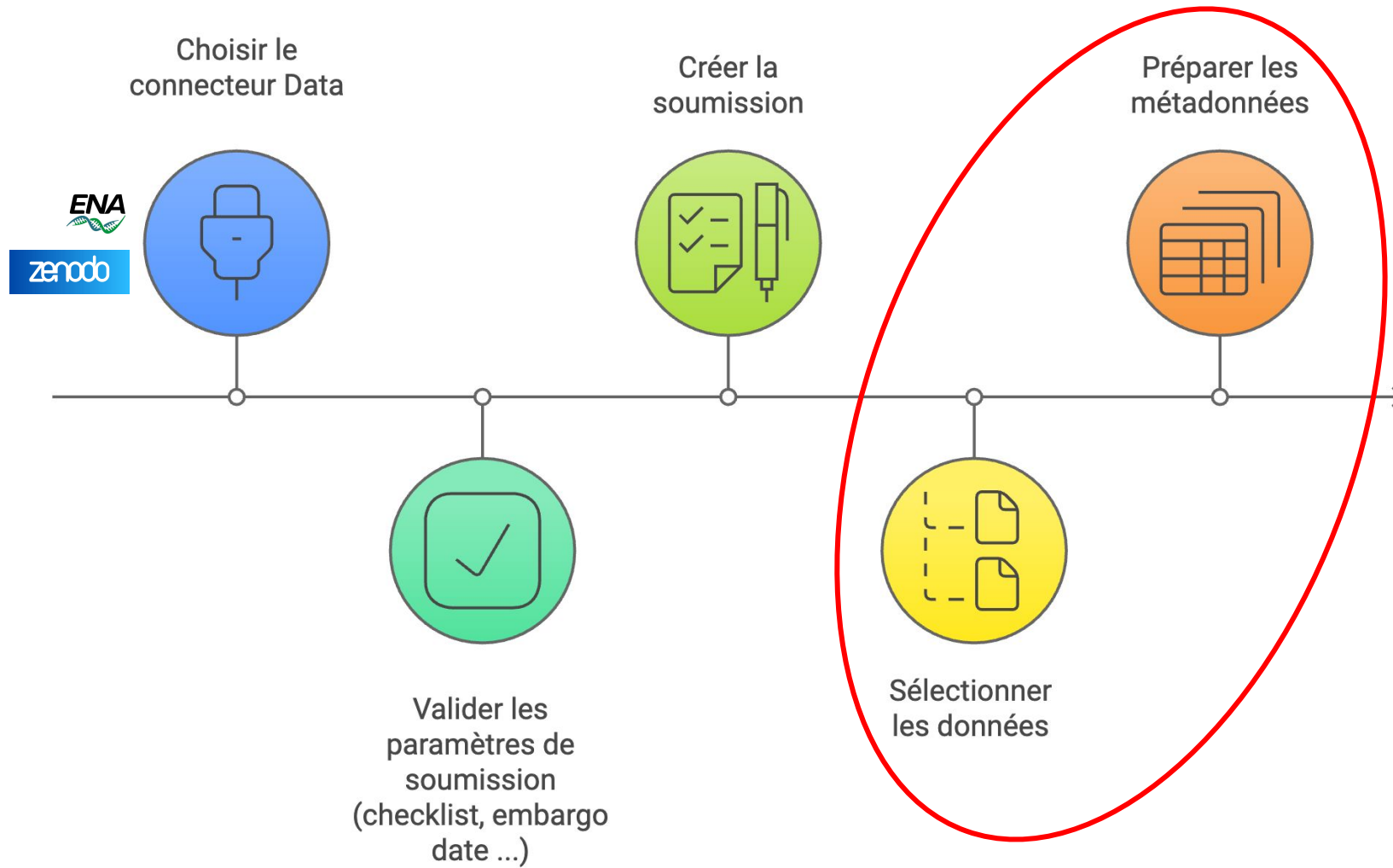
Des métadonnées peuvent être associées aux *Nodes*, *Samples*, *Data* et associations entre *Data*

The screenshot displays the MADBOT interface for editing a metadata record. The main content area shows the title "Growth control of the eukaryote cell: a systems biology study in yeast" and a detailed background text. Below the text, there are tabs for "DATALINKS", "SAMPLES", "METADATA", and "STUDY", with "METADATA" being the active tab. A table with columns "Field" and "Value" is shown, containing entries for "Library name", "Sample cell type", "Environmental sample", "Sample specie taxon", and "Common Name". A red error message is visible: "Sample specie taxon: must have required property 'scientificName'". The interface includes a sidebar with navigation options like "Dashboard", "Inbox", "Parameters", "Submissions", and "New investigation". At the bottom, there is a user profile for "Imane Messak" and a help icon.









Sélectionner
les données



The screenshot shows a 'File explorer' window with a breadcrumb path: Demo - Yeast Growth Control Systems B... / Growth control of the eukaryote cell... / Study of the impact of changes in flu... / protein expression profiling. The interface is divided into several panes: 'Nodes' (containing 'Growth control of th...', 'Study of the impact ...', and 'protein expressio...'), 'Data' (containing 'peptides.csv' and 'proteins.csv'), and a right-hand panel for 'protein expression profiling' (assay). The right panel includes an 'Information' section with the following details:

Information	
Created time	Fri, 06 Dec 2024 12:52:49 GMT
Last update time	Fri, 06 Dec 2024 12:52:49 GMT
Status	

A green button labeled 'SELECT (2)' is visible at the bottom right of the interface.

Processus de soumission - Exemple de l'ENA

Sélectionner les données



File explorer

Demo - Yeast Growth Control Systems B... / Growth control of the eukaryote cell... / Study of the impact of changes in flu... / protein expression profiling

Nodes: protein expressio...
Data: peptides.csv, proteins.csv

protein expression profiling
assay

Information

Created time	Fri, 06 Dec 2024 12:52:49 GMT
Last update time	Fri, 06 Dec 2024 12:52:49 GMT
Status	

SELECT (2)

ENA Submission for Yeast Study

Submission to ENA: draft

Everything saved | PARAMETERS | SUBMIT

DATA (2) | SUBMISSION ELEMENTS | ARTIFACTS | EXTERNAL IDS

ADD FILE

Filename	Location	Access	Connections	Actions
proteins.csv	Study of the impact of changes i... 🔗	Unreachable	Galaxy France Demo	⋮
Arabidopsis_thaliana.fasta	Study of the impact of changes i... 🔗	Accessible	Galaxy France	⋮

Items per page: 10 | 1-2 of 2 | < >

Préparer les métadonnées



IFB Core

- Inbox
- Settings & Members
- Dashboard
- Publications
 - > Node 1
 - v Node 2
 - > Sub node 1
 - > Sub node 2
 - > Node 3

New publication

Publication to ENA Draft Settings Publish

Data (1) general metadata Raw reads (1) Samples (1)

A raw read is a combination of a run and experiment

Name	Sample	Status	Actions
B35_Stretococcus_salivarius_genome	B35	Incomplete	

Processus de soumission - Exemple de l'ENA

Préparer les métadonnées



IFB Core

New publication Settings Publish

Publication to ENA Draft

Data (1) general metadata Raw reads (1) Samples (1)

A raw read is a combination of a run and experiment

Name	Sample	Status	Actions
B35_Stretococcus_salivarius_genome	B35	Incomplete	

IFB Core

New publication Settings Publish

Publication to ENA Draft

B35_Stretococcus_salivarius_genome

Field	value	Actions
Alias	B35_run_Stretococcus_salivarius_	
library layout	PAIRED	▼
forward raw sequence	B35_R1.fastq	▼
reverse raw sequence		
Instrument model		
Library source		
Library strategy		

C'est comment sous le capot ?








Un projet Open Source sous licence





Le **code source** est hébergé sur **Gitlab** : <https://gitlab.com/ifb-elixirfr/madbot>













Institut Français de Bioinformatique > Madbot

 **Madbot**  Group ID: 75576438  [Leave group](#)   [New project](#)

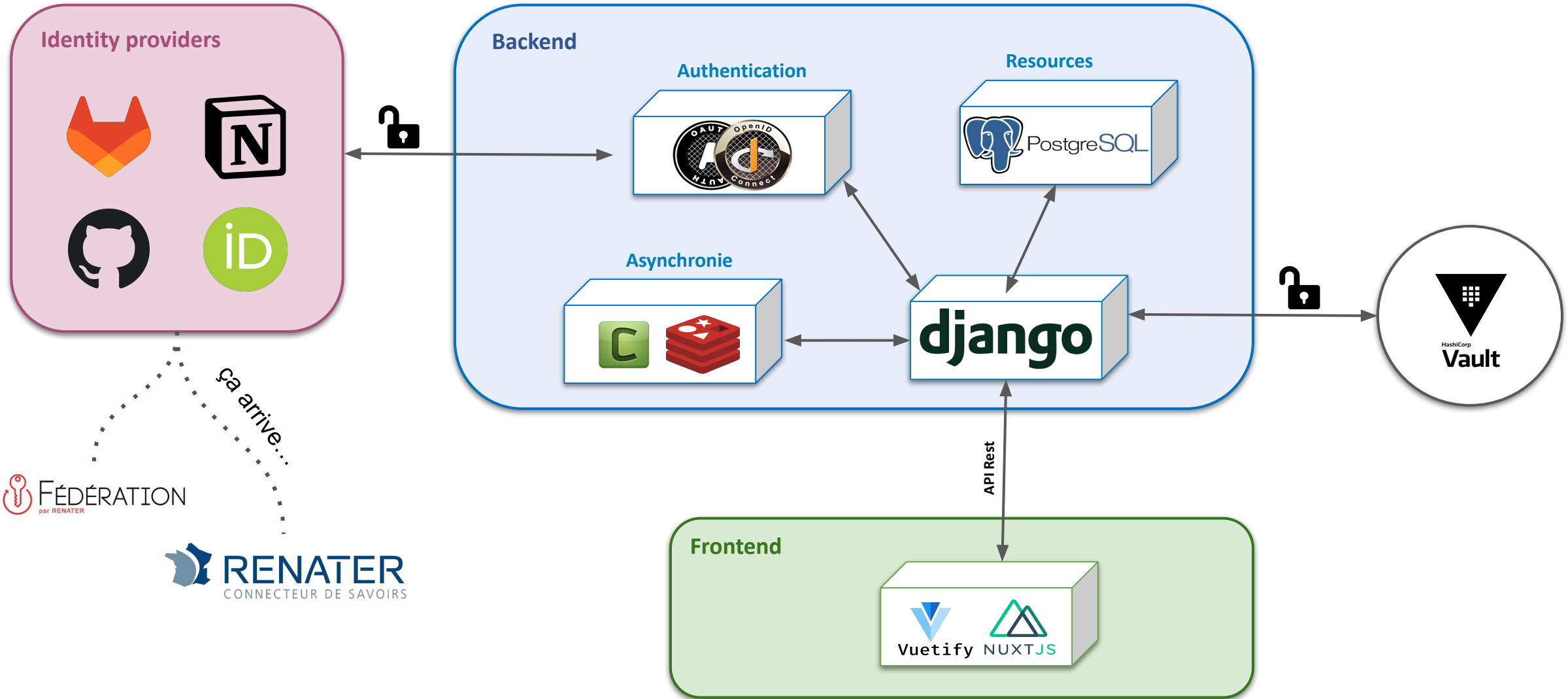
Subgroups and projects Shared projects Archived projects

Q Search

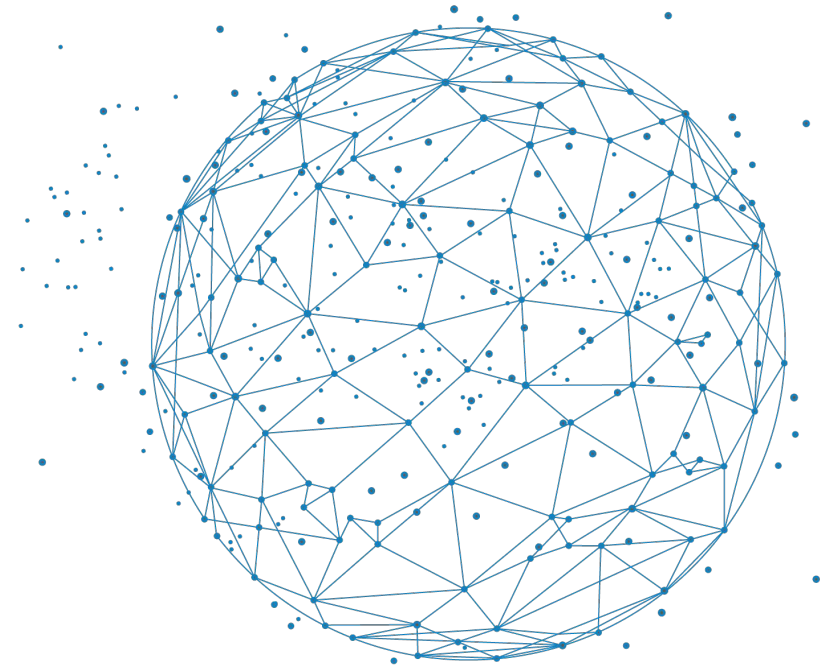
Name  

  Madbot API  API of Madbot, the Metadata And Data Brokering Online Tool  3 37 minutes ago
  Madbot Client  Web client for Madbot, the Metadata And Data Brokering Online Tool  1 4 days ago
  Madbot doc  Documentation for Madbot, the Metadata And Data Brokering Online Tool  3 6 days ago

Architecture

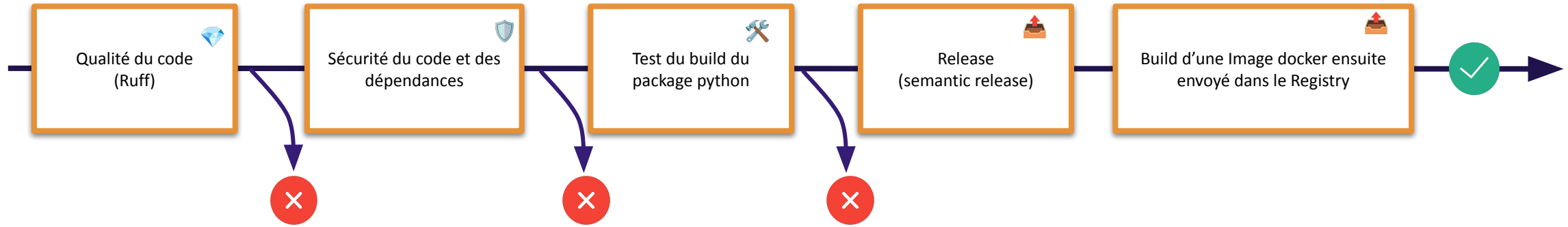


Un projet taillé pour la collaboration

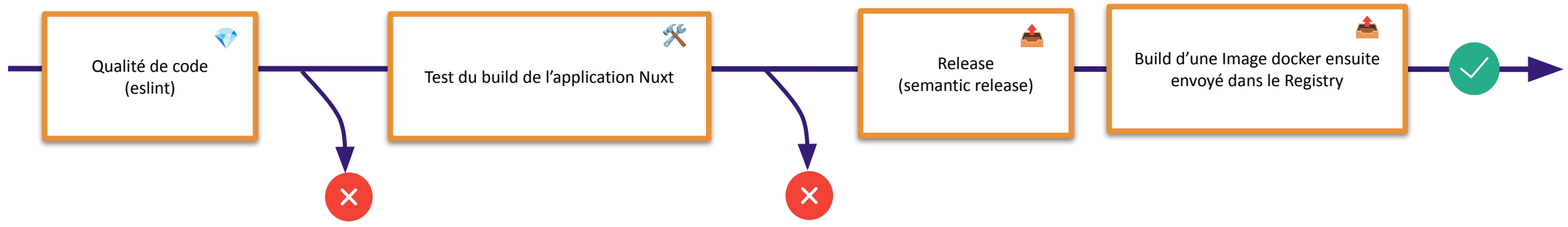




API



Client





Collaboration en cours

- Un groupe de travail se tient toutes les 3 semaines
- Collaboration avec l'action SOI et l'action M2
- Collaboration avec **Aubii** (UCA) pour la mise en place d'un environnement Docker
- Collaboration avec **FBI** pour la mise en place d'un connecteur IRODS/Omero
- Collaboration avec **Prose** (INRAE) pour la mise en place d'un connecteur DeepOmics

Collaboration à venir

- Collaboration avec l'action M4 pour la mise en place de formation et d'hackathon
- Et pourquoi pas vous ?





Merci pour votre attention

