bio.tools Documentation

Release latest

Dec 09, 2021

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This is the documentation for bio.tools.

Contents:

CHAPTER 1

What is bio.tools?

bio.tools is a portal to bioinformatics resources worldwide, aimed to help bioinformaticians and scientists:

- find, understand, compare and select resources == discovery
- use and connect them in workflows == (inter)operability

Our **vision** is to be the sustainable primary archive for basic tool metadata, providing a persistent reference to highquality (curated and verified) "canonical" descriptions of unique tools, with information about their provision via online services and various downloadable artefacts, and including entries for different versions of a tool, where these have major functional differences.

1.1 Objectives

Our main objectives are:

- build and maintain a comprehensive registry of high-quality software metadata / descriptions
- provide a web portal enabling registration, editing, search and discovery of the registry content
- support a **community** for the sustainable maintenance of the registry content and development of the portal features
- expose results of tool performance **benchmarking**, online service **monitoring** and other metrics of software and service quality
- integrate the registry with popular workbench environments in a way that improves resource interoperability
- · support registry stakeholders including tool providers and end-users

1.2 Scope

bio.tools scope is *application software* with well-defined data processing functions (inputs, outputs and operations). *bio.tools* includes a broad range of software types including tools available for immediate use as online services, or

in a form which which you can download, install, configure and run yourself. This includes simple tools with one or a few closely related functions, and complex, multimodal tools with many functions. It also includes executable workflows, database portals and Web APIs.

1.3 Technical components

- biotoolsSchema is a description model for bioinformatics software. It is a formalised XML schema (XSD) which defines 50 important scientific, technical and administrative attributes. It defines what attributes may be specified in a *bio.tools* entry, a precise syntax for those descriptions, and controlled vocabularies for consistent description of technical aspects such as software license and software type.
- EDAM ontology is an ontology of well-established, familiar concepts that are prevalent within bioinformatics and computational biology, including types of data and data identifiers, data formats, operations and topics. It defines precise semantics for the scientific description of software registered in *bio.tools*.
- Curation guidelines describe how each attribute should be specified, *i.e.* concern the quality of an entry. The guidelines go beyond the syntactic and semantic constraints defined by biotoolsSchema and EDAM, and are part of broader tool information standards being adopted by *bio.tools*.
- **Tool Cards** *e.g.* https://bio.tools/signalp provide key information at a glance for registered tools. Tool cards have human-friendly, persistent URLs which include the unique tool identifier ("signalp" in this case). The identifier is assigned upon registration is a URL-safe derivative of (normally identical to) the supplied tool name.
- **Query interfaces** available at https://bio.tools help *bio.tools* end-users with tool discovery and include the search bar, a compact "mini-card" view and a detailed "grid" view. See the Quickstart Guide.
- **Registration interface** enables manual creation of valid registry content and editing, including graphical editing via tabbed panes and an interactive JSON editor with inline error reporting. It is available to logged-on users via "Menu ... Add content". See the Quickstart Guide.
- bio.tools API provides programmatic means to query, add and edit registry content.
- **bio.tools metrics** available at https://bio.tools/stats include registry growth, contributors, annotation breakdown *etc.*

1.4 bio.tools Tool Identifiers

Each *bio.tools* entry is assigned a unique identifier (**biotoolsID**): a manually verified, URL-safe version of (normally identical to) the supplied tool name. The IDs are used in persistent URLs, resolving to Tool Cards of essential information. The recommended short-form is a compact URI (CURIE), which is resolvable in Identifiers.org.

	Example
biotoolsID	signalp
CURIE	biotools:signalp
Identifiers.org	http://identifiers.org/biotools/signalp
Tool Card URL	https://bio.tools/signalp

Registered software which, for one reason or another, is no longer operational, retain their ID and URL but are marked as obsolete. Hence, descriptions of legacy resources are archived.

1.5 Docs overview

- Contributors Guide how to get involved (please do!)
- Quickstart Guide quick guide on how to use the bio.tools user interfaces.
- Curators Guide how to create a high quality bio.tools entry.
- Editors Guide thematic editorships to improve *bio.tools* in scientific areas.
- Documentors Guide how to edit the *bio.tools* docs.
- API reference *bio.tools* API docs.
- Hangouts monthly coordination meetings (you're welcome to join!)
- Roadmap technical plans for the next year
- Studentships *bio.tools* studentship scheme for curation-focussed mini-projects.
- GitHub projects open projects of relevance to bio.tools.

bio.tools development is supported by ELIXIR - the European Research Infrastructure for life science information. *bio.tools* content is freely available to all under open license.

1.6 Getting involved : a quickstart guide

- 1. Read the docs but especially the contributors guide.
- 2. GitHub is used for task and issue tracking, see the bio.tools and EDAM organisations, in particuar the biotoolsregistry and edamontology projects. Email us if you want to join.
- 3. We run hangouts (coordination meetings) as required mostly for technical people routinely involved with *bio.tools* curation or software development. To suggest or join these calls email us.
- 4. Dive in at the deep end! There are no end of ongoing sub-projects and tasks to get involved with, see GitHub (at above links) or email us in the 1st instance to get orientated.

CHAPTER 2

Contributors Guide

2.1 bio.tools community site

GitHub is used for sharing code and data for all bio.tools-related projects:

- https://github.com/bio-tools/
- https://github.com/bio-tools/biotoolsschema
- https://github.com/bio-tools/biotoolsregistry
- https://github.com/edamontology/edamontology

2.2 Feature requests & issues

GitHub is used to track **fine-grained issues** and is the preferred way to make *bio.tools* feature requests, content suggestions, EDAM term requests, and bug reports:

- https://github.com/bio-tools/biotoolsregistry/issues
- https://github.com/bio-tools/biotoolsschema/issues
- https://github.com/edamontology/edamontology/issues

Note: GitHub is the primary means for technical coordination: collaborators are encouraged to browse tasks, review priorities, make comments and add new tasks.

2.3 Hangouts

Coordination meetings are organised as required. The hangouts usually have an open agenda and respond to current critical needs. Technical representatives of ELIXIR-DK institutes routinely attend and everyone is very welcome: if

you'd like to join email us.

2.4 Editing tool descriptions

You can contribute to *bio.tools* directly:

- register your own (or other people's) tools
- request edit rights (via a button on the bio.tools Tool Cards) on entries where tools are already registered
- request ownership (again via a button) of entries, if you are the developer of the tool described but it has been registerd by someone else
- ask for help via the email, especially in case you have many tools to add or edits to make

bio.tools benefits from the support of ELIXIR Nodes: collections of research institutes from a member country that provide the resources and services that are part of ELIXIR.

CHAPTER 3

Quickstart guide

This guide aims to help you through the different steps to add entries to bio.tools.

Note: If you find a bug, have any questions or suggestions, please get in touch.

3.1 Create an account

Creating an account on *bio.tools* is very quick and simple. Just click on the *Sign-up* button at the top-right corner of the page. Then you just need to give a username, your email address and a password to get your account done.

3.2 Add content

Everyone is welcome to add their own and other resources to *bio.tools*. Once your account is created, you can start adding your content by clicking on *Menu*... *Add content*.

The description of an new entry is handled by different tabs within the registration interface that are described below.

At any moment, you can check the validity of your information by clicking on Validate and save it by clicking on Save

Validate Save

Note: Saving the entry makes it directly available online. If you want to save what you have done without publishing it, the only way currently is to go to the *JSON* tab and save the .json file locally.

Important: The minimum information required (name, desription and homepage URL) is marked with a red asterix

in the registration interface.

It's recommended - especially if you have many tools to add - to read the Curators Guide first.

3.2.1 Summary

For this first part, you give the basic descriptors. This includess the **name** of your resource with a **description**, its **version** and a **homepage URL**. A unique **ID** is automatically generated from the name.

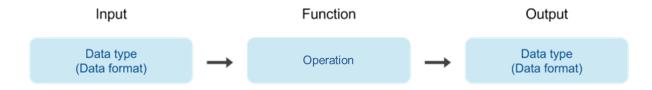
Note: A unique identifier (*bio.tools* toolID) is a URL-safe version of the supplied resource name. It's used in persitent URLs to *bio.tools* "Tool Cards", *e.g.* for the tool ID of "signalp":

- http://bio.tools/tool/signalp
- http://bio.tools/t/signalp
- http://bio.tools/signalp

Currently, if you want to change the ID you have to mail Registry Support. In future, the ID will be editable at registration time.

3.2.2 Function

This is where you describe the functionality of the tool based on the EDAM $ontology^1$. The functionality is captured in a diagram on the Tool Cards that look like this:



In each box, you can add as many fields as you want. You can also add a general comment about the function (*this is particularly useful when your entry has several functions*). It's highly recommended to read up about tool functions before filling this section.

Note: It can be difficult to find the right terms to describe a tools operation(s), input(s) or output(s). You can use OLS EDAM, BioPortal and EDAM Browser to browse EDAM and find the terms you need, or request new terms via GitHub. Improvements (including term requests) to the term picker in *bio.tools* are planned.

3.2.3 Labels

In this part, you can tell more about your tool:

- What type of resource it is (Command-line tool, Web application etc.)
- Relevant **topic**(s) the tool fits with (from the EDAM ontology¹).
- In which operating system it is possible to use it.

¹ Ison, J., Kalaš, M., Jonassen, I., Bolser, D., Uludag, M., McWilliam, H., Malone, J., Lopez, R., Pettifer, S. and Rice, P. (2013). EDAM: an ontology of bioinformatics operations, types of data and identifiers, topics and formats. Bioinformatics, 29(10): 1325-1332.

- The language used to develop the tool, its license and maturity.
- The accessibility of your tool and its cost.

You can also assign your tool to an arbitrary collection which can be useful for grouping together related tools.

3.2.4 Links

It is the place where your add links that do not belong to Download or Documentation. For instance, a link to a mailing list, mirror or repository (full list available on the drop-down menu of **Link type**).

3.2.5 Download

You can here share all the different download links you want. It can be many different kind such as binaries, source code, biological data, test data *etc*. (see the **Download type** drop-down menu).

3.2.6 Documentation

Make your different documentations for your tool available here. Again, you can assign type of documentation using **Documentation type**.

3.2.7 Publications

Share the different publications of the tool, which can be the primary publication (the one to cite when the tool is used), but also reviews or secondary references (see **Publication type**). You can use either the **PubMed Central ID** (PMCID), the **PubMed ID** (PMID) or the **Digital Object ID** (DOI) - DOI is preferred.

3.2.8 Credits & Support

Credits include all type of entities that contributed to the development, maintenance or provision of the resource. Credits can have an **Entity type** (Person, Institute *etc.*) and an **Entity role** (Developer, Documentor *etc.*). Use the role of *Primary contact* to indicate preferred contact details.

3.2.9 **JSON**

This is all the information you gave about your tool, formatted in JSON format.

3.2.10 Permissions

You can decide to make the entry either editable only by yourself, a list of users or anyone.

3.3 Update a resource

You'll see up to three different buttons at the bottom right of the Tool Card: Update this record >

- Click on Update this record to edit it
- Click on *Request editing rights* if you want to get edit rights to the entry
- Click on Request ownership if you want to claim ownership of the entry

..Note:: *bio.tools* entries are owned by the individuals who created them. Ownerships may grant edit rights, or transder ownership of their entries to others.

3.4 Remove a resource

From the tool card, click on update this record. Then you can remove the entry by clicking on the remove button

Warning: Removing an entry is definitive. There's no way back (other than emailing Registry Support).

3.5 Search for a tool

Coming soon...

3.6 References

CHAPTER 4

Curators Guide

Attention:

- guidelines for bio.tools curators, including EDAM annotation guidelines.
- to make suggestions about these guidelines please add comments via GitHub
- · for curation advice mail registry-support

bio.tools includes all types of bioinformatics *tools* - application software with well-defined data processing functions (inputs, outputs and operations). This ranges from simple tools with a single primary function, to complex, multimodal tools with many disinct functions. Tools may be available for immediate use as online services, or in a form which you can download, install, configure and run yourself.

Usually, a *bio.tools* entry describes a discrete tool. Some entries describe *collections* of tools, such as software suites. The scope, *i.e.* the types of tools that may be included, and the attributes for their description, are defined in biotoolsS-chema which uses the EDAM ontology as a source of terms for the tool scientific description. These curation guidelines describe how to create a high quality tool description, above and beyond the syntactic and semantic constraints that are defined in biotoolsSchema and EDAM.

- general guidelines include basic considerations, annotation of tool functions and the use of EDAM. You should read these first of all.
- guidelines on specific attributes defined in the biotoolsSchema
- guidelines specific to individual types of tools

The key words "MUST", "MUST NOT", "REQUIRED", "SHALL", "SHALL NOT", "SHOULD", "SHOULD NOT", "RECOMMENDED", "MAY", and "OPTIONAL" in this document are to be interpreted as described in RFC 2119:

- "MUST", "REQUIRED" or "SHALL" mean that the guideline is an absolute requirement of the specification.
- "MUST NOT" or "SHALL NOT" mean that the guideline is an absolute prohibition of the specification.
- "SHOULD" or "RECOMMENDED" mean that there may exist valid reasons in particular circumstances to ignore a particular guideline, but the full implications must be understood and carefully weighed before doing so.

- "SHOULD NOT" or the phrase "NOT RECOMMENDED" mean that there may exist valid reasons in particular circumstances when acting contrary to the geuideline is acceptable or even useful, but the full implications should be understood and the case carefully weighed before doing so.
- "MAY or "OPTIONAL" mean that the guideline is truly optional; you can choose to follow it or not.

Note: The guidelines are a key component of an emerging information standard for tools being adopted by *bio.tools*, as a basis to monitor content and label *bio.tools* entries.

- automatically verified guidelines are (or will be) checked via automated periodic QC of the bio.tools system
- **manually verified** guidelines are checked *via* manual QC performed by trusted curators (*bio.tools* admin, entry owners *etc.*)
- advice given in boxes (notes, tips, caution etc. are not verified

4.1 General guidelines

4.1.1 Before you start

Consider the following *before* creating a *bio.tools* entry:

- 1. Are one or more entries required to describe the software?
 - workbenches and other suites often require multiple entries.
 - tools with multiple interfaces (*e.g.* Command-line tool, Web API, Web service and Web application) **SHOULD** be described by a single entry **unless** these interfaces provide fundamental functional differences (see Tool functions below).
 - if in doubt, mail registry-support.
- 2. What tool types apply?
 - one or more tool types may be assigned in a single entry reflecting different facets of the software described by the entry.
 - read the tool type-specific guidelines before you create the tool.
- 3. What if the software is already registered?
 - if you're the rightful owner of the entry (*i.e.* the tool developer or provider of an online service) then request ownership of it
 - otherwise, request edit rights

Make these requests using the buttons at the bottom of the Tool Card (see *e.g.* https://bio.tools/signalp).

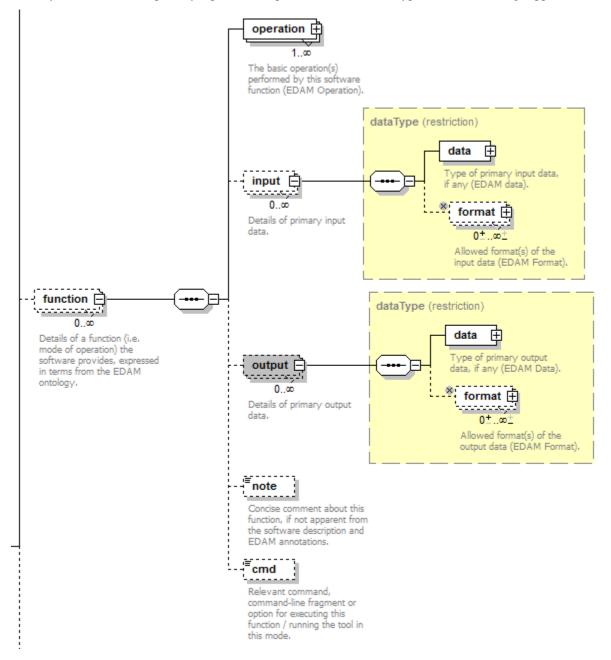
If you plan to register multiple entries en masse, please discuss this first with bio.tools admin.

4. Are there version-specific considerations?

- as a rule, a *bio.tools* entry **SHOULD** describe the *latest version* available at the time of registration and **SHOULD** be updated, as required, for subsequent releases.
- if a new version has fundamental functional differences (see Tool functions below) it **MAY** be registered as an entirely new entry. In such cases, follow carefully the guidelines for tool name and version annotations.
- 5. Plan how to describe the tool functions.
- 6. Read the general EDAM annotations guidelines.

4.1.2 Tool functions

bio.tools uses a model of software (see below) defined within biotoolsSchema. A tool can have one or more basic functions (modes of operation), each function performing one or more specific operation (e.g."Sequence alignment"), and may have one or more primary inputs and outputs, each of a defined type of data and listing supported format(s).



Plan how how to describe the software:

- identify the distinct functions (modes of operation) and the individual operations associated with each one. Typically different functions (modes) perform different operations and for well documented tools, this is usually obvious. If in any doubt mail registry-support.
- as a general rule, if the tool allows an option between doing one thing or another, then you **MUST** annotate the operations as distinct functions. If in contrast a tool always does one or more things, then you **MUST** annotate

these as distinct operations within a single function.

- *bio.tools* aims for fairly coarse-grained description, *i.e.* you **SHOULD** only specify the primary functions and operations, from a typical end-user perspective. If a tool happens to perform some operation internally, but this is secondary to its advertised purpose, then you **SHOULD NOT** annotate it. If in doubt mail registry-support
- this holds for input and output too, *e.g.* a sequence alignment tool would be annotated as reading sequences (input), and writing a sequence alignment (output), but not with gap insertion and extension penalties, or other parameters.
- many tools allow a primary input or output to be specified in a number of alternative ways, *e.g.* a sequence input that may be specified *via* a sequence identifier, or as a literal sequence. In such cases, you **MAY** annotate the alternatives as distinct functions (see above). If specifying just one alternative, you **SHOULD** use the EDAM Data concept for the type of data, rather than identifier.

Note: A future refactoring may improve the modelling for alternative specification of inputs and outputs, by allowing multiple data+format couplets for a given input or output. If this is done, the proposed guideline would be:

- you MAY annotate all the commonly used alternatives and, if specifying alternatives, MUST annotate these as distinct data + format couplets within a single input or output.
- many inputs and outputs are complex, with individual data files containing multiple types of data. You **MUST** select the single EDAM Data term that best describes an input or output (see EDAM annotations below) and **MUST NOT** specify multiple EDAM Data terms describing differents facets of the data.

Input on this issue is welcomed via GitHub.

4.1.3 EDAM annotations

The EDAM ontology is used to annotate applicable topics, operations, and the type and format of inputs and outputs. The general guidelines below apply for all EDAM annotations.

- **1. MUST NOT** use "organisational" EDAM concepts *e.g.* Topic of "Topic" or Operation of "Operation" (see note below)
- 2. SHOULD use the most specific term(s) available, bearing in mind some concepts are necessarily overlapping or general. If multiple sibling terms are applicable (*i.e.* terms under a common parent), the parent term may be applicable.
- 3. SHOULD NOT use both a term and it's parent or other ancestor, when annotating a single attribute. An exception would be a tool which *e.g.* performs some general Sequence analysis operations but specialises on Protein feature detection.

Tip: If you're struggling to find the terms you need, or the meaning of a term is not obvious, search EDAM using the browsers below (they have different functionalities). Multiple searches using synonyms, alternative spellings *etc.* can help.

- EBI OLS browser
- NCBO BioPortal browser
- EDAM ontology browser from IFB
- EDAM Tool Annotator Demo

If you cannot find the right term, request it's added to EDAM via GitHub but first read the guidelines on how to request a term.

Note: It currently takes some time from requesting new EDAM terms for these to be supported in *bio.tools*. In future, you'll be able to request terms directly via the *bio.tools* registration interface and these terms will become immediately available for use, albeit subject to approval and possible change before inclusion in EDAM and *bio.tools*.

Note: Some high-level "organisational" concepts defined in EDAM are intended primarily to structure the hierarchy, and are not intended for annotation in *bio.tools*. They are defined in EDAM.owl via "<usageGuideline>Not recommended for annotation in bio.tools.</usageGuideline>'. Such tips are visible in the OLS and BioPortal browsers.

4.2 Attribute guidelines

Guidelines below are organised into sections as they appear in the bio.tools registration user interface

4.2.1 Summary group

Basic information about the software.

Name (tool)

Canonical software name assigned by the software developer or service provider, e.g. "needle"

- 1. MUST use name in common use, *e.g.* in the tool homepage and publication.
- 2. MUST use short form if available e.g. ExPASy not ExPASy Bioinformatics Resource Portal.
- **3. MUST NOT** include general or technical terms ("software", "application", "server", "service", "SOAP", "REST", "RESTful" *etc.*) *unless* these are part of the common name
- **4. MUST NOT** misappropriate the names of other tools, *e.g.* there are many online BLAST services besides the original NCBI BLAST tool; calling any of them "BLAST" would be wrong
- 5. MUST NOT include version or status information including terms like "alpha", "beta" etc. unless this is part of common name
- 6. SHOULD preserve capitalisation *e.g.* ExPASy not expasy.
- 7. SHOULD follow the naming patterns (see below)

Note:

• see the syntax guidelines.

Note: Naming patterns

For database portals use the pattern:

```
name (acronym) e.g. The Protein Databank (PDB)
```

- a common abbreviation can be given instead of an acronym
- if no common acronym or abbreviation exists, omit this part: do not invent one!

For tools that simply wrap or provide an interface to some other tool, including Web APIs (REST), Web services (SOAP+WSDL), and web applications over command-line tools, use the pattern:

```
{collectionName} toolName {API|WS}{( providerName)} e.g. EMBOSS water
API (ebi)
```

where:

- collectionName is the name of suite, workbench or other collection the underlying tool is from (if applicable)
- toolName is the canonical name of the underlying tool
- use API for Web APIs or WS for Web services
- providerName is the name of the institute providing the online service (if applicable)

If in exceptional cases (*i.e.* when registering, as separate entries, versions of a tool with fundamental differences), substitute for toolName in the pattern above:

toolname versionID e.g. FindPeaks 3.1

where versionID is the version number.

Tip:

- in case of mulitple related entries be consistent, e.g. Open PHACTS and Open PHACTS API
- be wary of names that are very long (>25 characters). If shortening the name is necessary, don't truncate it in a way (*e.g.* within the middle of a word) that would render it meaningless or unintuitive

Description

Textual description of the software, e.g. "needle reads two input sequences and writes their optimal global sequence alignment to file. It uses the Needleman-Wunsch alignment algorithm to find the optimum alignment (including gaps) of two sequences along their entire length. The algorithm uses a dynamic programming method to ensure the alignment is optimum, by exploring all possible alignments and choosing the best."

- 1. MUST provide a concise summary of purpose / function of the tool
- 2. MUST begin with a capital letter and end with a period ('.')
- **3. SHOULD NOT** include any of the following, *unless* essential to distinguish the tool from other bio.tool entries:
 - provenance information e.g. software provider, institute or person name
 - describe how good the software is (mentions of applicability are OK)
- 4. SHOULD NOT include URLs
- 5. SHOULD NOT include DOIs

Note:

• see the syntax guidelines.

Homepage

Homepage of the software, or some URL that best serves this purpose, e.g. "http://emboss.openbio.org/rel/rel6/apps/needle.html"

- 1. MUST resolve to a web page from the developer / provider that most specifically describes the tool
- 2. SHOULD NOT specify an FTP site unless nothing else is available.
- 3. MAY specify a repository if no better alternative is available.

Note:

• see the syntax guidelines.

Tip: In case a tool lacks it's own website, a URL of it's code repository is OK. Do not use a general URL such as an institutional homepage, unless nothing better is available.

Version (tool)

Version information (typically a version number) of the software applicable to this bio.tools entry, e.g. "6.4.0.0"

- 1. MUST correctly identify the tool version as described by the other attributes (see note below)
- 2. MUST specify exactly the public version label in common use
- **3. MUST NOT** include tokens such as "v", "ver", "version", "rel", "release" *etc.*, *unless* these are part of the public version label
- 4. MAY identify all tool versions which are applicable to the entry
- 5. MAY specify a version for database portals and web applications, but only if this is used in the common name

Note:

• see the syntax guidelines.

Important:

Care is needed to ensure annotations correspond to the indicated tool version.

- **only** change the version if you're sure there's no fundamental change to the specified tool functions (operations, inputs and outputs)
- if there are fundamental changes, update the tool function annotation
- do not assume version "1" in case the version number is not readily findable

Tip: One or more version fields may be specified, and each - in princple - allows flexible specification of version information including single versions, ranges, lists and lists including ranges, *e.g.*:

- 1.1
- beta01

- 2.0 2.7
- 1.1, 1.2.1, 1.4, v5
- 1.1 1.4, 2.0-alpha, 2.0-beta-01 2.0-beta-04, 2.0.0
- *etc*.

We recommend to keep things simple (one version label per field by default) and pragmatic (using version ranges where desirable).

Other IDs

A unique identifier of the software, typically assigned by an ID-assignment authority other than bio.tools, e.g. "RRID:SCR_015644"

- 1. MUST correctly identify the same tool as indicated by the biotoolsID
- 2. MUST include version information if IDs for multiple different versions are specified
- 3. MAY specify the type of identifier (see below)

Туре	Description
doi	Digital Object Identifier of the software assigned (typically) by the software developer or
	service provider.
rrid	Research Resource Identifier as used by the NIH-supported Resource Identification Portal
	(https://scicrunch.org/resources).
сре	Common Platform Enumeration (CPE) identifier as listed in the CPE dictionary (https://
	//cpe.mitre.org/dictionary/).
biotoolsCURIE	bio.tools CURIE (secondary identifier).

Note:

• see the syntax guidelines.

Attention: Alternative IDs of type biotoolsCURIE are set (and can only be changed) by *bio.tools* admin. They allow *bio.tools* to support multiple biotoolsIDs (hence resolvable Tool Card URLs) for a single tool; this done in exceptional circumstances only, *e.g.* the name of a tool is changed.

Value

Value of tool identifier, e.g. "RRID:SCR_001156"

• 1. MUST specify a valid identifier for the tool.

Type (otherID)

Type of tool identifier, e.g. "rrid"

• **1. MAY** specify the applicable type, in terms from a controlled vocabulary (see below) - although this should not normally be necessary

Version (otherID)

Version information (typically a version number) of the software applicable to this identifier, e.g. "1.4"

- 1. MUST correctly identify the applicable tool version
- 2. MUST follow the general guidelines for version

4.2.2 Function group

Details of a function (i.e. mode of operation) the software provides, expressed in concepts from the EDAM ontology.

Operation

The basic operation(s) performed by this software function (EDAM Operation), e.g. "'Protein signal peptide detection' (http://edamontology.org/operation_0418)"

- **1. MUST** correctly specify operations performed by the tool, or (if version is indicated), those specific version(s) of the tool
- 2. MUST be correctly organised into multiple functions, in case the tool has multiple modes of operation (see guidelines for tool functions).
- **3. SHOULD** describe all the primary operations performed by that tool and **SHOULD NOT** describe secondary / minor operations: if in any doubt, mail registry-support.

Attention:

• see the general guidelines for EDAM annotations.

Note:

• see the syntax guidelines.

Data type (input and output data)

Type of primary input / output data (if any) e.g. "'Sequence' (http://edamontology.org/data_2044)"

- 1. MUST correctly specify types of input or output data processed by the tool, or (if version is indicated), those specific version(s) of the tool
- 2. MUST be correctly associated with the operation(s); for each function in case the tool has multiple modes of operation (see guidelines for tool functions).
- **3. SHOULD** describe all the primary inputs and outputs of the tool and **SHOULD NOT** describe secondary / minor inputs and outputs: if in any doubt, mail registry-support.

Attention:

• see the general guidelines for EDAM annotations.

Tip:

• many tools allow a primary input to be specified in a number of alternative ways, the common case being a sequence input that may be specified via a sequence identifier, or by typing in a literal sequence. In such cases, annotate the input using the EDAM Data concept for the type of data, not the identifier.

Note:

• see the syntax guidelines for input and output

Data format (input and output data)

Allowed format(s) of primary inputs/outputs e.g. "'FASTA' (http://edamontology.org/format_1929)"

- 1. MUST correctly specify data formats supported on input or output by the tool, or (if version) is indicated, those specific version(s) of the tool
- 2. MUST be correctly associated with the data type of an input or output (see guidelines for tool functions).
- **3. SHOULD** describe the primary data formats and **MAY** exhaustively describe *all* formats: if in any doubt, mail registry-support.

Attention: see the general guidelines for EDAM annotations.

Note:

• see the syntax guidelines.

Note (function)

Concise comment about this function, if not apparent from the software description and EDAM annotations, e.g. "This option is slower, but more precise."

- 1. MUST not duplicate what is already apparent from the EDAM annotations
- 2. SHOULD be concise and summarise only critical usage information
- 3. SHOULD NOT duplicate online documentation; give a link if necessary

Note:

• see the syntax guidelines.

Command

Relevant command, command-line fragment or option for executing this function / running the tool in this mode, e.g "-s best"

• 1. MUST specify precisely a command, command-line fragment or option specified in the tool documentation

• 2. MUST be correctly associated with a function (the command must be used to invoke that specific tool function)

Note:

• see the syntax guidelines.

4.2.3 Labels group

Miscellaneous scientific, technical and administrative details of the software, expressed in terms from controlled vocabularies.

Tool type

The type of application software: a discrete software entity can have more than one type, e.g. "Command-line tool, Web application"

• 1. MUST specify all types that are applicable, in terms from a controlled vocabulary (see below)

Туре	Description
Bioinformatics por- tal	web site providing a platform/portal to multiple resources used for research in a focused area, including biological databases, web applications, training resources and so on.
Command-line tool	A tool with a text-based (command-line) interface.
Database portal	A Web application, suite or workbench providing a portal to a biological database.
Desktop application	A tool with a graphical user interface that runs on your desktop environment, <i>e.g.</i> on a PC or mobile device.
Library	A collection of components that are used to construct other tools. bio.tools scope includes component libraries performing high-level bioinformatics functions but excludes lower-level programming libraries.
Ontology	A collection of information about concepts, including terms, synonyms, descriptions etc.
Plug-in	A software component encapsulating a set of related functions, which are not standalone, <i>i.e.</i> depend upon other software for its use, <i>e.g.</i> a Javascript widget, or a plug-in, extension add-on etc. that extends the function of some existing tool.
Script	A tool written for some run-time environment (<i>e.g.</i> other applications or an OS shell) that automates the execution of tasks. Often a small program written in a general-purpose languages (<i>e.g.</i> Perl, Python) or some domain-specific languages (<i>e.g.</i> sed).
SPARQL endpoint	A service that provides queries over an RDF knowledge base via the SPARQL query lan- guage and protocol, and returns results via HTTP.
Suite	A collection of tools which are bundled together into a convenient toolkit. Such tools typ- ically share related functionality, a common user interface and can exchange data conve- niently. This includes collections of stand-alone command-line tools, or Web applications within a common portal.
Web application	A tool with a graphical user interface that runs in your Web browser.
Web API	An application programming interface (API) consisting of endpoints to a request-response message system accessible via HTTP. Includes everything from simple data-access URLs to RESTful APIs.
Web service	An API described in a machine readable form (typically WSDL) providing programmatic access via SOAP over HTTP.
Workbench	An application or suite with a graphical user interface, providing an integrated environment for data analysis which includes or may be extended with any number of functions or tools. Includes workflow systems, platforms, frameworks etc.
Workflow	A set of tools which have been composed together into a pipeline of some sort. Such tools are (typically) standalone, but are composed for convenience, for instance for batch execution via some workflow engine or script.

Tip:

• in cases where a given software is described by more than one entry (*e.g.* a web application and its API are described separately) then assign only the types that are applicable to that entry.

Note:

- *bio.tools* includes all types of bioinformatics tools: application software with well-defined data processing functions (inputs, outputs and operations). When registering a tool, one or more tool types may be assigned, reflecting the different facets of the software being described.
- see the syntax guidelines.

Topic

General scientific domain the software serves or other general category (EDAM Topic), e.g. "'Protein sites, features and motifs' (http://edamontology.org/topic_3510)"

- 1. MUST specify the single most important and relevant scientific topic
- 2. MAY specify all highly relevant scientific topics
- 3. SHOULD NOT exhaustively specify all the topics of lower or secondary relevance

Attention:

• see the general guidelines for EDAM annotations.

Note:

• see the syntax guidelines.

Operating system

The operating system supported by a downloadable software package, e.g. "Linux"

• 1. MUST specify all operating systems that are applicable, in terms from a controlled vocabulary (see below)

Operating system	Description
Linux	All flavours of Linux/UNIX operating systems.
Windows	All flavours of Microsoft Windows operating system.
Mac	All flavours of Apple Macintosh operating systems (primarily Mac OS X).

Note:

• see the syntax guidelines.

Programming language

Name of programming language the software source code was written in, e.g. "C"

- 1. MUST specify the primary language used, in terms from a controlled vocabulary (see below)
- 2. MAY exhaustively specify other languages used

Programming language
ActionScript
Ada
AppleScript
Assembly language
AWK
Bash

Continued on next page

Programming language
C
C#
C++
COBOL
ColdFusion
CWL
D
Delphi
Dylan
Eiffel
Forth
Fortran
Groovy
Haskell
Icarus
Java
JavaScript
JSP
LabVIEW
Lisp
Lua
Maple
Mathematica
MATLAB
MATLAD MLXTRAN
NMTRAN
OCaml
Pascal
Perl
PHP
Prolog
PyMOL
Python
R
Racket
REXX
Ruby
SAS
Scala
Scheme Shell
Smalltalk
SQL Turing
Turing
Verilog
VHDL Viewel Parie
Visual Basic
XAML Other

Table 1 – continued from previous page

Note:

• see the syntax guidelines.

License

Software or data usage license, e.g. "GPL-3.0"

- 1. MUST acurately describe the license used.
- 2. SHOULD use "Proprietary" in cases where the software is under license (not defined in biotoolsSchema) whereby it can be obtained from the provider (*e.g.* for money), and then owned, *i.e.* definitely not an open-source or free software license.
- **3. SHOULD** use "Freeware" for software that is available for use at no monetary cost. In other words, freeware may be used without payment but may usually not be modified, re-distributed or reverse-engineered without the author's permission.
- 4. SHOULD use "Not licensed" for software which is not licensed and is not "Proprietary".
- **5. SHOULD** use "Other" if the software is available under a license not listed by biotoolsSchema and which is not "Proprietary".
 - a controlled vocabulary of valid terms is defined in biotoolsSchema.
 - see the syntax guidelines.

Tip:

• Use the "Other" license for custom institutional licenses that are out of scope of biotoolsSchema. If you've found a license that you think should be included in biotoolsSchema please report it *via* GitHub.

Note: Most permisible values are identifiers from the SPDX license list (https://spdx.org/licenses/). In future, based on the specified license a label (e.g. "Open-source") may be attached to the *bio.tools* entry (see table below)

License	Description
Open-source	Software is made available under a license approved by the Open Source Initiative (OSI).
	The software is distributed in a way that satisfies the 10 criteria of the Open Source Defini-
	tion maintained by OSI (see https://opensource.org/docs/osd). The source code is available
	to others.
Free software	Free as in 'freedom' not necessarily free of charge. Software is made available under a
	license approved by the Free Software Foundation (FSF). The software satisfies the criteria
	of the Free Software Definition maintained by FSF (see http://www.gnu.org/philosophy/
	free-sw.html). The source code is available to others.
Free and open	Software is made available under a license approved by both the Open Source Initia-
source	tive (OSI) and the Free Software Foundation (FSF), and satisfies the criteria of the OSI
	Open Source Definition maintained (https://opensource.org/docs/osd) and the FSF Free
	Software Definition (http://www.gnu.org/philosophy/free-sw.html). Such software ensures
	users have the freedom to run, copy, distribute, study, change and improve the software.
	The source code is available to others.
Copyleft	Software is made available under a license designated as 'copyleft' by the Free Soft-
	ware Foundation (FSF). The license ensures such software is free and that all modi-
	fied and extended versions of the program are free as well. Free as in 'freedom' not
	necessarily free of charge, as per the Free Software Definition maintained by FSF (see
	http://www.gnu.org/philosophy/free-sw.html).

Table 2: Labelling based on license (future work)

Collection

Unique ID of a collection that the software has been assigned to within bio.tools, e.g. "CBS

• 1. SHOUD be short and intuitive

Tip:

• collections may be created for for any arbitrary purpose

Note:

• see the syntax guidelines.

Maturity

How mature the software product is, e.g. "Mature"

• 1. MUST acurately reflect the software maturity, in terms from a controlled vocabulary (see below)

Maturity	Description
Emerging	Nascent or early release software that may not yet be fully featured or stable.
Mature	Software that is generally considered to fulfill several of the following: secure, reliable, actively maintained, fully featured, proven in production environments, has an active community, and is described or cited in the scientific literature.
Legacy	Software which is no longer in common use, deprecated by the provider, superseded by other software, replaced by a newer version, is obsolete etc.

Attention:

• normally only the developer or provider of a tool is sure of its maturity. If you are not sure, then do not complete this field.

Note:

• see the syntax guidelines.

Cost

Monetary cost of acquiring the software, e.g. "Free of charge (with retritions)"

• 1. MUST acurately describe the monetary cost of acquiring the software, in terms from a controlled vocabulary (see below)

Cost	Description
Free of charge	Software which available for use by all, with full functionality, at no monetary cost to the
	user.
Free of charge (with	Software which is available for use at no monetary cost to the user, but possibly with limited
restrictions)	functionality, usage restrictions, or other limitations.
Commercial	Software which you have to pay to access.

Note:

• see the syntax guidelines.

Accessibility

Whether there are non-monetary restrictions on accessing an online service., e.g. "Open access"

• 1. MUST acurately describe the accessibility conditions that apply, in terms from a controlled vocabulary (see below)

Accessibility	Description
Open access	An online service which is available for use to all, but possibly requiring user accounts /
	authentication.
Open access (with	An online service which is available for use to all, but possibly with some usage limitations
restrictions)	and other restrictions.
Restricted access	An online service which is available for use to a restricted audience, e.g. members of a
	specific institute.

Note:

• see the syntax guidelines.

ELIXIR Platform

Name of the ELIXIR Platform that is credited, e.g. "Tools"

• **1. MUST** only credit the ELIXIR Platform if directly contributing to the work, using a term from a controlled vocabulary (see below)

ELIXIR Platform	Description
Data	ELIXIR Data Platform
Tools	ELIXIR Tools Platform
Compute	ELIXIR Compute Platform
Interoperability	ELIXIR Interoperability Platform
Training	ELIXIR Training Platform

ELIXIR Node

Name of the ELIXIR Node that is credited, e.g. "Norway"

• 1. MUST only credit the ELIXIR Node if directly contributing to the work, using a term from a controlled vocabulary (see below)

ELIXIR Node
Belgium
Czech Republic
Denmark
EMBL
Estonia
Finland
France
Germany
Greece
Hungary
Ireland
Israel
Italy
Luxembourg
Netherlands
Norway
Portugal
Slovenia
Spain
Sweden
Switzerland
UK

ELIXIR Community

Name of relevant ELIXIR (or associated) community, e.g. "Galaxy"

• **1. MAY** cite any ELIXIR Community to which the software is directly relevant.

ELIXIR Community
3D-BioInfo
Federated Human Data
Galaxy
Human Copy Number Variation
Intrinsically Disordered Proteins
Marine Metagenomics
Metabolomics
Microbial Biotechnology
Plant Sciences
Proteomics
Rare Diseases

4.2.4 Link group

Miscellaneous links for the software e.g. repository, issue tracker or mailing list.

Note:

- the *bio.tools* registration interace & API allows a curator to record when a link of a certain type is known to *not* be available
- see the syntax guidelines.

URL (link)

A link of some relevance to the software (URL), e.g. "https://github.com/pharmbio/sciluigi/issues"

- 1. MUST resolve to a page of the indicated link type
- 2. MUST NOT give a general link (e.g. homepage URL) if a more specific link is available

Link type

The type of data, information or system that is obtained when the link is resolved, e.g. "Mailing list"

- **1. MUST** acurately specify the type of information available at the link, in terms from a controlled vocabulary (see below)
- 2. MUST use type "Other" if another, more specific type is not available
- 3. SHOULD specify all the types that are applicable

Link type	Description		
Discussion forum	Online forum for user discussions about the software.		
Galaxy service	An online service providing the tool through the Galaxy platform.		
Helpdesk	A phone line, web site or email-based system providing help to the end-user of the software.		
Issue tracker	Tracker for software issues, bug reports, feature requests etc.		
Mailing list	Mailing list for the software announcements, discussions, support etc.		
Mirror	Mirror of an (identical) online service.		
Software catalogue	Some registry, catalogue etc. other than bio.tools where the tool is also described.		
Repository	A place where source code, data and other files can be retrieved from, typically via plat-		
	forms like GitHub which provide version control and other features, or something simpler,		
	e.g. an FTP site.		
Social media	A website used by the software community including social networking sites, discussion		
	and support fora, WIKIs etc.		
Service	An online service (other than Galaxy) that provides access (an interface) to the software.		
Technical monitor-	Information about the technical status of a tool.		
ing			
Other	Other type of link for software - the default if a more specific type is not available.		

Note (link)

Comment about the link, e.g. "Please use the issue tracker for reporting bugs and making features requests."

• 1. SHOULD be a concise summary of practical information

4.2.5 Download group

Links to downloads for the software, e.g. source code, virtual machine image or container.

Note:

- the *bio.tools* registration interace & API allows a curator to record when a documentation link of a certain type is known to *not* be available
- see the syntax guidelines.

URL (download)

Link to download (or repo providing a download) for the software, e.g. "http://bioconductor/packages/release/bioc/src/contrib/VanillaICE_1.36.0.tar.gz"

- **1. MUST** resolve to a page providing either an immediately download, or links for a download of the indicated link type
- 2. MUST NOT give a general link (e.g. homepage URL) if a more specific link is available

Download type

Type of download that is linked to, e.g. "Binaries"

• 1. MUST acurately specify the type of download available at the link, in terms from a controlled vocabulary (see below)

- 2. MUST use type "Other" if another, more specific type is not available
- **3. SHOULD** use type "Downloads page" for links to general downloads pages (*i.e.* one which includes details about multiple types of download)

Download type	Description	
API specification	File providing an API specification for the software, e.g. Swagger/OpenAPI, WSDL RAML file.	
Biological data	Biological data, or a web page on a database portal where such data may be downloaded.	
Binaries	Binaries for the software; compiled code that allow a program to be installed without having to compile the source code.	
Command-line	File providing a command line specification for the software.	
specification		
Container file	Container file including the software.	
Icon	Icon of the software.	
Screenshot	Screenshot of the software.	
Source code	The source code for the software, that can be compiled or assembled into an executable	
	computer program.	
Software package	A software package; a bundle of files and information about those files, typically including	
	source code and / or binaries.	
Test data	Data for testing the scientific performance of the software or whether it is working correctly.	
Test script	Script used for testing testing whether the software is working correctly.	
Tool wrapper	Tool wrapper in Common Workflow Language (CWL) format for the software.	
(CWL)		
Tool wrapper	Galaxy tool configuration file (wrapper) for the software.	
(galaxy)		
Tool wrapper (tav-	Taverna configuration file for the software.	
erna)		
Tool wrapper	Workbench configuration file (other than taverna, galaxy or CWL wrapper) for the software.	
(other)		
VM image	Virtual machine (VM) image for the software.	
Downloads page	Web page summarising general downloads available for the software.	
Other	Other type of download for software - the default if a more specific type is not available.	

Note (download)

Comment about the download, e.g. "Complete distibution"

• 1. SHOULD be concise and summarise only practical information about the link

Version (download)

Version information (typically a version number) of the software applicable to this download.

- 1. MUST correctly identify the applicable tool version
- 2. MUST follow the general guidelines for version

4.2.6 Documentation group

Links to documentation about the software e.g. user manual, API documentation or training material.

Note:

- the *bio.tools* registration interace & API allows a curator to record when a documentation link of a certain type is known to *not* be available
- see the syntax guidelines.

URL (documentation)

Link to documentation on the web for the tool, e.g. "http://bioconductor.org/packages/release/bioc/html/VanillaICE.html"

- 1. MUST resolve to a page of the indicated documentation type
- 2. MUST NOT give a general link (e.g. homepage URL) if a more specific link is available

Documentation type

Type of documentation that is linked to, e.g. "Citation instructions"

- 1. MUST acurately specify the type of documentation available at the link, in terms from a controlled vocabulary (see below)
- 2. MUST use type "Other" if another, more specific type is not available
- 3. SHOULD specify all the types that are applicable

Documentation	Description
type	
API documentation	Human-readable API documentation.
Citation instructions	Information on how to correctly cite use of the software; typically which publication(s) to
	cite, or something more general, e.g. a form of words to use.
Code of conduct	A set of guidelines or rules outlining the norms, expectations, responsibilities and proper
	practice for individuals working within the software project.
Command-line op-	Information about the command-line interface to a tool.
tions	
Contributions	Information about policy for making contributions to the software project.
policy	
FAQ	Frequently Asked Questions (and answers) about the software.
General	General documentation.
Governance	Information about the software governance model.
Installation instruc-	Instructions how to install the software.
tions	
Quick start guide	A short guide helping the end-user to use the software as soon as possible.
Release notes	Notes about a software release or changes to the software; a change log.
Terms of use	Rules that one must agree to abide by in order to use a service.
Training material	Online training material such as a tutorial, a presentation, video etc.
User manual	Information on how to use the software, tailored to the end-user.
Other	Some other type of documentation not listed in biotoolsSchema.

Note (documentation)

Comment about the documentation, e.g. "Comprehensive usage information suitable for biologist end-users."

• 1. SHOULD be concise and summarise only practical information about the link

4.2.7 Relation group

Details of a relationship this software shares with other software registered in bio.tools.

- 1. MUST correctly identify a relationship between two bio.tools entries
- 2. MUST NOT not contradict a relationship that is already specified in *bio.tools*
- 3. MUST specify a valid biotoolsID (of a tool that's registerd in *bio.tools*)

Note:

• see the syntax guidelines.

biotoolsID (relation)

bio.tools ID of an existing bio.tools entry to which this software is related, e.g. "needle"

Relation type

Type of relation between this and another registered software, e.g. "isNewVersionOf"

Relation type	Description
isNewVersionOf	The software is a new version of an existing software, typically providing new or improved
	functionality.
hasNewVersion	(inverse of above)
uses	The software provides an interface to or in some other way uses the functions of other
	software under the hood, e.g. invoking a command-line tool or calling a Web API, Web
	service or SPARQL endpoint to perform its function.
usedBy	(inverse of above)
includes	A workbench, toolkit or workflow includes some other, independently available, software.
includedIn	(inverse of above)

4.2.8 Publication group

Publications about the software

- 1. MUST correctly identify a relevant publication
- 2. MUST specify multiple IDs for a single publication within a single publication group
- 3. SHOULD specify a DOI (if available) (in preference to PMID and PMCID)
- 4. MAY specify one or more types that match the publication

Note:

• see the syntax guidelines.

PubMed Central ID

PubMed Central Identifier (PMCID) of a publication about the software, e.g. "PMC4343077"

PubMed ID

PubMed Identifier (PMID) of a publication about the software, e.g. "21959131"

Digital Object ID

Digital Object Identifier (DOI) of a publication about the software, e.g. "10.1038/nmeth.1701"

Publication type

Type of publication, e.g. "Primary"

- 1. MUST acurately specify the type of publication, in terms from a controlled vocabulary (see below)
- 2. SHOULD specify all the types that are applicable

Publication type	Description
Primary	The principal publication about the tool itself; the article to cite when acknowledging use
	of the tool.
Method	A publication describing a scientific method or algorithm implemented by the tool.
Usage	A publication describing the application of the tool to scientific research, a particular task
	or dataset.
Benchmarking	A publication which assessed the performance of the tool.
study	
Review	A publication where the tool was reviewed.
Other	A publication of relevance to the tool but not fitting the other categories.

Note (publication)

A comment about the publication, e.g. "A comparison of the software to others performing a similar function."

- 1. SHOULD be concise and acurate, elaborating on the motivation, purpose *etc.* of the publication
- 2. SHOULD NOT duplicate information that is, or can, be provided via the type or other attributes, *i.e.* do not specify "Review article", "Cite this where the software is used" *etc.*

Version (publication)

Version information (typically a version number) of the software applicable to this publication.

- 1. MUST correctly identify the applicable tool version
- 2. MUST follow the general guidelines for version

4.2.9 Credit group

Individuals or organisations that should be credited, or may be contacted about the software.

- 1. SHOULD provide contact details for the first port-of-call when seeking help with the software, and SHOULD annotate the role of this entity as "Primary contact"
- 2. MAY specify one or more other credits

Note:

- a credit consists of the name, email and/or URL of some entity that is credited, with other associated metadata
- see the syntax guidelines.

Name (credit)

Name of the entity that is credited, e.g. "EMBL EBI"

- 1. MUST give the first and last names of a person, or the correct name of some other entity.
- 2. MUST NOT give a redirect, *e.g.* "See publication", a URL, or any information other than the name of the entity that is credited.

ORCID ID

Unique identifier (ORCID iD) of a person that is credited, e.g. "http://orcid.org/0000-0002-1825-0097"

• 1. MUST correctly identify a credited person

Note: Open Researcher and Contributor IDs (ORCID IDs) provide a persistent reference to information on a researcher, see http://orcid.org/.

GRID ID

Unique identifier (GRID ID) of an organisation that is credited, e.g. "grid.5170.3"

• 1. MUST correctly identify a credited organisation

Note: Global Research Identifier Database IDs (GRID IDs) provide a persistent reference to information on an organisation, see https://www.grid.ac/.

ROR ID

Unique identifier (ROR ID) of an organisation that is credited, e.g. "03yrm5c26"

• 1. MUST correctly identify a credited organisation

Note: Research Organization Registry (ROR) IDs provide a persistent reference to information on research organisations, see https://ror.org/.

FundRef ID

Unique identifier (FundRef ID or Funder ID) of a funding organisation that is credited, e.g. "10.13039/100009273"

• 1. MUST correctly identify a credited organisation

Note: The Funder Registry (formerly FundRef) IDs provide a persistent reference to information on funding organisations registered in the Crossref registry, see https://www.crossref.org/services/funder-registry/.

Email

Email address of the entity that is credited e.g. "hnielsen@cbs.dtu.dk"

- 1. MUST specify a syntactically valid email address
- 2. MUST NOT specify an email address that is not publicly acknowledged as credit for the software, *e.g.* on a webpage or in a publication
- 3. MUST NOT specify a stale (obsolete) email address

URL (credit)

URL for the entity that is credited, e.g. homepage of an institute, e.g. "http://www.ebi.ac.uk/"

• 1. MUST resolve to a page of information directly relevant to the credited entity

Entity type

Type of entity that is credited, e.g. "Person"

• 1. MUST acurately specify the type of entity that is credited, in terms from a controlled vocabulary (see below)

Entity type	Description
Person	Credit of an individual.
Project	Credit of a community software project not formally associated with any single institute.
Division	Credit of or a formal part of an institutional organisation, e.g. a department, research group,
	team, etc
Institute	Credit of an organisation such as a university, hospital, research institute, service center,
	unit etc.
Consortium	Credit of an association of two or more institutes or other legal entities which have joined
	forces for some common purpose. Includes Research Infrastructures (RIs) such as ELIXIR.
Funding agency	Credit of a legal entity providing funding for development of the software or provision of
	an online service.

Entity role

Role performed by entity that is credited, e.g. "Developer"

- 1. MUST acurately specify the primary role of credited entity, in terms from a controlled vocabulary (see below)
- 2. MAY exhaustively specify all the roles of the credited entity

Role	Description
Developer	Author of the original software source code.
Maintainer	Maintainer of a mature software providing packaging, patching, distribution etc.
Provider	Institutional provider of an online service.
Documentor	Author of software documentation including making edits to a bio.tools entry.
Contributor	Some other role in software production or service delivery including design, deployment,
	system administration, evaluation, testing, documentation, training, user support etc.
Support	Provider of support in using the software.
Primary contact	The primary point of contact for the software.

Note (credit)

A comment about the credit, e.g. "Wrote the user manual."

- 1. SHOULD be concise and acurate, elaborating on the contribution of the credited entity
- 2. MUST NOT duplicate information that is, or can, be provided via the role attribute, *i.e.* do not specify only "Developer", "Support" *etc.*

4.2.10 Community group

Community and external partner resources linked from bio.tools.

The community and external partner resources have their own custom properties in bio.tools to facilitate integration between bio.tools and other resource providers.

If you're a resource provider and would like to integrate with bio.tools please email registry-support@elixir-dk.org or create an issue on our GitHub page.

4.2.11 BioLib Annotations (Community)

BioLib is a platform for biological data science applications. With BioLib apps, you can run bioinformatics tools directly in your web browser.

See more details at https://biolib.com.

- 1. MUST specify a valid BioLib App name
- 2. MUST specify a valid BioLib Author username
- 3. MUST specify the Author name

App name (BioLib)

Application Name of an existing BioLib app, e.g. "MyBioTool".

Author username (BioLib)

BioLib Username of the user that created the BioLib app, e.g. "example-university"

Author name (BioLib)

The display name of the author that created the BioLib app, e.g. "The Example University".

4.3 Tool type guidelines

4.3.1 Bioinformatics portal

A web site providing a platform/portal to multiple resources used for research in a focused area, including biological databases, web applications, training resources and so on.

- pick one or more topics that best describe the portal content.
- consider carefully whether the portal will be described by a single, or more than one *bio.tools* entry (see Before you start). Where the portal aggregates one or more discrete tools (web applications), databases *etc.*, it is recommended to register these as separate entries.

4.3.2 Command-line tool

A tool with a text-based (command-line) interface.

• carefully identify the major functions (modes of operation) performed by the tool (see Tool functions) and annotate the major operation(s) associated with each function, in turn.

4.3.3 Database portal

A Web application, suite or workbench providing a portal to a biological database.

- pick one or more topics that best describe the database content. See also the specialised Data management concepts.
- consider carefully whether the database portal will be described by a single, or more than one *bio.tools* entry (see Before you start). In case the portal contains one or more discrete tools (web applications), it is recommended to register these as separate entries.
- consider an operation of Database search (or its children)

4.3.4 Desktop application

A tool with a graphical user interface that runs on your desktop environment, e.g. on a PC or mobile device.

- desktop applications often have complex functionality: carefully identify the major functions (modes of operation) performed by the application (see Tool functions) and annotate the major operation(s) associated with each function, in turn.
- consider an operation of Visualisation (or its children) typical of desktop apps.

4.3.5 Library

A collection of components that are used to construct other tools. bio.tools scope includes component libraries performing high-level bioinformatics functions but excludes lower-level programming libraries.

- in case the library includes just a few components, each should (typically) be modelled as a distinct function (see Tool functions); annotate the major operation(s) associated with each component (function) in turn.
- in case the library includes very many components, model the whole library as having a single function (see Tool functions); and annotate only the major operation(s) (do not try to be exhaustive).

4.3.6 Ontology

A collection of information about concepts, including terms, synonyms, descriptions etc.

- pick Ontology and terminology and one or more most relevant topics describing the scope of the ontology.
- do not annotate the function (operations, or type / format of the input and output data)

4.3.7 Plug-in

A software component encapsulating a set of related functions, which are not standalone, *i.e.* depend upon other software for its use, e.g. a Javascript widget, or a plug-in, extension add-on etc. that extends the function of some existing tool.

- when annotating the plug-in function(s), be careful to not duplicate the description of the tool which plug-in plugs into
- carefully identify the major new functions (modes of operation) which the plug-in provides, and annotate the major operation(s) associated with each function, in turn.

4.3.8 Script

A tool written for some run-time environment (e.g. other applications or an OS shell) that automates the execution of tasks. Often a small program written in a general-purpose languages (e.g. Perl, Python) or some domain-specific languages (e.g. sed).

- scripts typically have a single function (mode of operation) (see Tool functions), however, in case of complex scripts, carefully identify the major functions (modes of operation) performed by the script, and annotate the major operation(s) associated with each function, in turn.
- · pick one or more most relevant topics

4.3.9 SPARQL endpoint

A service that provides queries over an RDF knowledge base via the SPARQL query language and protocol, and returns results via HTTP.

- pick the operation of "Query and retrieval" (http://edamontology.org/operation_0224)
- do not annotate the type or format of the input and output data

4.3.10 Suite

A collection of tools which are bundled together into a convenient toolkit. Such tools typically share related functionality, a common user interface and can exchange data conveniently. This includes collections of standalone command-line tools, or Web applications within a common portal.

• pick one or more most relevant topics that describe the workbench as a whole (don't try to be exhaustive)

- describe the attributes that are common to the suite as a whole, not (typically) attributes of individual tools
- · individual tools included in the suite should be registered as separate entries
- when annotating the operation of the suite, select operations that are core function of the suite itself / common to all tools in the suite. Alternatively pick one or two of the primary operation(s) of the included tools
- entries for the suite itself and it's component tools can be associated by annotatong them as part of a common collection

Tip: If you are considering to register a suite with many tools, it is a good idea to discuss this first with the bio.tools admin.

Attention: do not annotate the type and 'format <>'_ of input and output data, *unless* all tools in the suite happen to have these in common

4.3.11 Web application

A tool with a graphical user interface that runs in your Web browser.

· pick one or more most relevant topics

Note:

• for software that essentially just wraps or provides an interface to some other tool, *e.g.* a web application or web service over an existing tool, use the pattern toolName providerName where providerName is a name (without spaces) of some institute, workbench, collection *etc.*, *e.g.* cufflinks cloudIFB. **Do not** misappropriate the original name!

4.3.12 Web API

An application programming interface (API) consisting of endpoints to a request-response message system accessible via HTTP. Includes everything from simple data-access URLs to RESTful APIs.

- pick one or more most relevant topics
- in general, describe the attributes of the API as a whole, not individual endpoint of the API (see note below)
- in case the API has a single endpoint only, the input(s), operation(s) and output(s) may be annotated
- in case the API has many endpoints, annotate the primary operation(s), but **not** the inputs and outputs
- annotate the location of machine-readable API specification (*e.g.* openAPI file) using the download attribute with download type of API specification annotate the location of any human-readable documentation using the documentation attribute with documentation type of API specification
- when assigning the name, use the pattern name API e.g. Open PHACTS API
- in case the web service provides an interface to an existing tool registered in *bio.tools*, try to ensure the relevant annotations are consistent

Note:

• biotoolsSchema includes a basic model of an API specification including endpoints however this is not yet supported in *bio.tools*

4.3.13 Web service

An API described in a machine readable form (typically WSDL) providing programmatic access via SOAP over HTTP.

- · pick one or more most relevant topics
- in general, describe the attributes of the web service as a whole, not individual endpoint of the service (see note below)
- in case the web service has a single endpoint only, the input(s), operation(s) and output(s) may be annotated
- in case the web service has many endpoints, annotate the primary operation(s), but **not** the inputs and outputs
- annotate the location of the WSDL file using the download attribute with download type of API specification
- annotate the location of any human-readable documentation using the documentation attribute with documentation type of API specification
- when assigning the name, use the pattern name WS e.g. EMMA WS
- in case the web service provides an interface to an existing tool registered in *bio.tools*, try to ensure the relevant annotations are consistent

Note:

• biotoolsSchema includes a basic model of an API specification including endpoints however this is not yet supported in *bio.tools*

4.3.14 Workbench

An application or suite with a graphical user interface, providing an integrated environment for data analysis which includes or may be extended with any number of functions or tools. Includes workflow systems, platforms, frameworks etc.

- pick one or more most relevant topics that best describe the workbench as a whole (don't try to be exhaustive)
- describe the attributes of the workbench as a whole, not (typically) individual tools or functions provided by it
- individual tools included in the workbench, especially where these tools are independently available, should be registered as separate entries
- individual functions provided by the workbench, especially where these are not independently available, should each be described in their own function
- entries for the workbench itself and it's component tools can be associated by annotatong them as part of a common collection

Tip: If you are considering to register a complicated workbench with many tools or functions, it is a good idea to discuss this first with the *bio.tools* admin.

4.3.15 Workflow

A set of tools which have been composed together into a pipeline of some sort. Such tools are (typically) standalone, but are composed for convenience, for instance for batch execution via some workflow engine or script.

- pick one or more most relevant topics that best describe the workflow as a whole (don't try to be exhaustive)
- when deciding how to annotate a workflow inputs, operations and outputs, consider the worfklow as a "black box", *i.e.* annotate the input(s) to, output(s) from and primary operation(s) of the workflow as a whole

Note:

• bio.tools does not currently contain many examples of workflows. We welcome input on how to describe worfklows and ensure good coverage: please get in touch with us.

Important: workflows can contain many tools; **do not** list all the operations performed by these tools, just the main operation(s) of the workflow as a whole.

4.4 Further guidelines (bio.tools admin only)

Attention: The guidelines that follow are for attributes and other aspects under the control of *bio.tools* admin. If you're not a *bio.tools* admin you can ignore this section.

4.4.1 summary->biotoolsID

Unique ID (case insensitive) of the tool that is assigned upon registration of the software in bio.tools, normally identical to tool name, e.g. "needle".

Attention:

- the ID by default is a URL-safe version of the tool name and can only be changed by bio.tools admin.
- MUST use the default value where possible
- MUST be clean and intuitive (in case use of default is not possible)
- MUST NOT truncate the name (in the middle of a word, or at all) if this renders the ID ugly or meaningless

Note: Transformation rules

The following rules apply when transforming the supplied tool name:

- replace ' ' (spaces) in the name with underscores (a single underscore in case of multiple spaces)
- preserve all reserved characters (uppercase and lowercase letters, decimal digits, hyphen, period, underscore, and tilde), but remove other characters
- use '_' to delimit parts of names but only if these are not already truncated in the original name
- can only start with letters or numbers
- cannot end with a . (dot) character

• adhere to the same patterns for tool name, e.g. EMBOSS_water_API_ebi

4.4.2 summary->biotoolsCURIE

bio.tools CURIE (compact URI) based on the unique bio.tools ID of the tool, e.g. "biotools:needle"

Note:

• identical to biotoolsID but with the prefix biotools:

4.4.3 credit->elixirNode

ELIXIR node credited for developing or providing the software - the software is in Node Service Delivery Plan, e.g. "Denmark"

- 1. MUST acurately specify an ELIXIR Node that is credited, in terms from a controlled vocabulary
- 2. MUST only be credited on tools that are in a Node's Service Delivery Plan.
- 3. MUST only be set by a an ELIXIR Node manager or ELIXIR Hub.

4.4.4 credit->elixirPlatform

ELIXIR platform credited for developing or providing the software, e.g. "Tools"

- 1. MUST acurately specify an ELIXIR Platform that is credited, in terms from a controlled vocabulary
- 2. MUST only be set by a an ELIXIR Node manager or ELIXIR Hub.

CHAPTER 5

Domains in bio.tools

bio.tools domains provide a way to "slice" the bio.tools content into subsets of tools.

The name **"domain"** (or sometimes also referred as **"subdomain"**) comes from the fact that after creation the domains can be accessed via regular URL subdomains in bio.tools such as proteomics.bio.tools or rare-diseases.bio.tools.

The advantage of creating and using bio.tools domains is that you can describe, link to, and search within a smaller subset (or "slice") of the bio.tools content which can help with the description and findability of tools relevant to a specific task.

Examples of bio.tools domains include:

- tools related to a specific bioinformatics area such as Proteomics, Rare diseases, COVID etc
- a subset or a collection of tools developed or used by a research group, lab or any other entity
- any other grouping, subset or collection of tools that serves a specific purpose or provides a certain value to researchers, curators, developers, tool users etc

A domain in bio.tools is a collection of tools along with metadata describing the domain itself. The metadata of the domain contains the following attributes:

5.1 Domain properties

5.1.1 Domain name

The unique name (or identifier) of a domain.

Note: the domain name can only be provided at the time of the domain creation. After the domain has been created the name cannot be changed,

- **REQUIRED** field: the domain name is the only metadata field required to create a bio.tools domain
- MUST be URL-safe, clean and intuitive
- MUST be related to the tools in the domain

5.1.2 Domain title

The title of the domain.

• MUST be concise and descriptive. The domain title will appear at the top part of the domain page

5.1.3 Domain subtitle

The subtitle of the domain.

• **SHOULD** be a longer version of the domain title. Not always needed as any other long description will be present in the **domain description** field

5.1.4 Domain tags

Tags associated with a domain.

• MUST be keywords that help with the search and discovery of the domain

5.1.5 Domain collections

Collections associated with the domain.

When inputing a domain collection the user is presented with suggestions for tool collections. Domain collections are used as a matching mechanism between tools and domains. See the **Priate vs Public domains** section below for more.

5.1.6 Domain description

Longform description of the domain.

SHOULD contain any descriptive text about the domain that does not fit in any of the above fields.

Domain descriptions offer support for simple HTML tags such as **bold**, *italics* or anchor tags.

5.1.7 Domain resources

Domain resources provide the tool content of the domain. Any tool entry in bio.tools can be added to a domain.

A user can search for a tool by name, identifier, collection or credit entities.

Tools can be added or removed from a domain at any time. The tool content of a domain can change if a domain is public, see the **Private vs Public domains** section below.

MUST contain tools relevant to the domain

5.1.8 Private domain flag

Indicates if the domain is private (true by default) to a user or public to the bio.tools registry.

5.2 Private vs Public domains

5.2.1 Private domains

With private domains only the creator of the domain can change the tools that belong to that specific domain. By default domains are private. This option is recommended when full control of the domain content is required.

5.2.2 Public domains

A public domain is a domain in which other users can populate that domain by tagging tools with the same collections that are also present for that domain. If a domain is tagged with certain collections and tools are also tagged with the same collections then that tool will be added to the domain. In this way users can tag their tools as part of domains without needing permissions to that domain.

Even if users can modify the tool content of a specific domain they cannot change the metadata of the domain (e.g. domain title, domain description etc)

5.3 Explore domains

All domains in bio.tools can be viewed and searched at https://bio.tools/domains or going to Explore -> Domains in the bio.tools page header.

5.4 Create a domain

In order to create a domain a user needs a bio.tools account and to be logged in. In the bio.tools page header go to Menu -> Manage domains or directly to https://bio.tools/domain-manager.

This page will show all the domains (if any) a user has created. To create a new domain click on the *Add* button. This will take you to the domain create page. Fill in the fields described above (*only domain name required*) and click Save at the bottom right. This will validate and create your domain and redirect to the domain update page where tools can also be added to the domain.

5.5 Update a domain

From the domain manager page click on the *Edit* button for any existing domains to update domain metadata or to add / remove tools associated to a domain.

5.5.1 Add-Remove tools

Tools can only be added after a domain has been created, on the domain update page. In the "*Search for tools*" section of the page use the searchbox to find the tools to add to the domain. Tools can be searched by tool name, tool identifier, tool collection and credits. Click on the Search button to find relevant tools. Results will appear below the searchbox. Add a tool by clicking the *Add to domain* button for a single tool or click *Add all tools* to add all tool results to the domain.

The tools added to the domain will show up below in the *Tools included the domain* section. In this section any included tools can also be removed.

Click the "Update" button at the bottom to save your changes.

CHAPTER 6

Community-specific guidelines

Tool information profiles and tutorials tailored to specific communities

Different communities - whether national, scientific or ones focused on a specific project - have different perspectives on the information they wish to disseminate about the tools and services within their portfolios.

Tool information profiles are a formal way to define which tool attributes - supported by the bio.tools registry - should be specified within a set of tool descriptions registered in *bio.tools*.

Accompanying the profiles are tutorials which tool developers and service providers can follow to improve the description of their resources in bio.tools. The aim is to improve the quality of the community tools portfolio, by improving the *bio.tools* entries, and by highlighting areas where the service around those tools can be improved.

Note: This page currently describes the profile and tutorial developed for IFB, but the expectation is that other communities will follow.

6.1 IFB tools

Caution: This tutorial describes some features of *bio.tools* which have not yet been released in the public version available at https://bio.tools. These features - and what to do - are indicated in an "Caution" box (like this one).

These instructions will guide you through the steps to register your tools and databases in bio.tools and describe them to the standard required for inclusion in the next iteration of the IFB Catalogue - the French national catalogue of bioinformatics resources.

There are various sources of information and help:

• *This document* provides guidelines tailored to the IFB catalogue, highlighting key information and common pitfalls.

- The bio.tools Curators Guide provides in-depth curation guidelines. You might need to refer to it, wherever you see the {learn more} links.
- The biotoolsSchema documentation summarises the attributes, information model and controlled vocabularies including the EDAM ontology - used by bio.tools. Links to these docs are provided where needed.
- To get help using *bio.tools*, or for general curation advice, please mail registry-support.
- If you have questions specifically about the IFB catalogue curation process, you can mail Jon Ison directly.

Note: These instructions are tailored to the needs of IFB tool providers. If you find a bug, or have any questions or suggestions, please post them on GitHub.

6.1.1 1. Get a bio.tools account

You'll need an account to create *bio.tools* entries or edit existing ones. Creating an account is simple: just go to

Sign-up bio.tools and click on at the top-right corner of the page.

You'll be asked for a username, email address and password. Your account will be setup immediately.

Note: *bio.tools* entries are owned by the individuals who created them. Owners may grant edit rights, or transfer ownership of their entries to other registered users. The rightful owner of a *bio.tools* entry is usually the person who developed the tool, or provides an online service, but it can be some other responsible person, e.g. a dedicated curator.

6.1.2 2. Claim your bio.tools entries

As a software developer or service provider, you should own the *bio.tools* entries describing your tools, by claiming ownership of existing entries or creating new ones.

You'll need to login first, by clicking on



at the top-right corner of the page.

To see whether a tool is already registered, search for it by its name. Simply type the name in the search box. You may need to click on the Name facet to narrow-down the search:

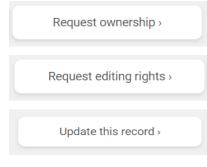
	tools/t?ord=desc	Q 🛧 🔟 Q O 🖸 🖉 🛆 🚥 🔜 🌄 🚭			
Apps ★ Bookmarks 🤡	Journal access 💁 Mail – EFoster@swa 🙇 ClassDojo 🥥 DTU Mail 💽 Completed				
elizir	signal	13524 tools About Login Sign-up			
<i>Chia tools</i> Sort by Update	Everything Topic Operation Input Output Tool type Langu: Accessibility Cost License Credit Collection <u>Name</u>	age 1. Display as Compact Detailed			
	signalAlign				
Ocean Gene Atla:	Atlas of Cancer Signalling Network (ACSN)				
The Ocean Gene A	MetaboSignal	: gene sequence catalogs (ENA), sample environmental			
context (PANGAEA of either a sequence	LnSignal	reads onto gene catalogs). User queries are composed ince alignment. Homologs of the user query in the gene			
catalogs are identif	bam signal s	their read based estimated abundance are displayed in			
interactive maps ar as known homolog	Signal-CF	hin its context of marine environmental homologs as well			
us known normolog	Signal-3L				
Ecology Marin	eSIGNAL				
Dhuda ann atla tara					
Phylogenetic tree	SignalP	alignment Quantification Map drawing			

Once you find your entry you can go ahead and update it. If you can't find the entry, you'll need to create it.

Important: All tools that were submitted for consideration in the ELIXIR FR Service Delivery Plan should already be registered, but may have only very basic details. You will need to take ownerhsip and improve the entries. Before starting work, please ensure you understand the *information requirement* and follow the *guidelines* below.

Updating entries

To edit an existing entry, you need to click through to the Tool Card for the tool in question, *e.g.* https://bio.tools/ signalp. You'll see a one or two buttons at the bottom right of the Tool Card, depending on whether you're logged in, and own the entry or not.

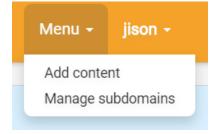


- Click on Request ownership if you want to claim ownership of the entry
- Click on Request editing rights if you want to edit rights on the entry, but not own it
- Click on *Update this record* to edit the entry (visible only if you own the entry or have editing rights)

Note: It can take a little while for other users to respond to requests for edit rights or ownership. If these are not granted within a day or two, please mail registry-support.

Creating entries

To create new entries you'll need to be logged onto bio.tools. Click on Menu ... Add content:



bio.tools editing interface

The *bio.tools* editing interface helps you to create valid tool descriptions. It's organised into different tabs (*Summary*, *Function*, *Labels etc.*):

🕲 bio.tools x +	- • ×
$\leftarrow \rightarrow$ C \triangle \triangleq bio.tools/signalp/edit	a 🖈 🔟 🕒 🖉 🙆 📟 🚃 🖏 😓 🗎 🍎 🗄
🗰 Apps ★ Bookmarks 📀 Journal access 🧕 Mail - B	EFosterülswa 🙇 ClassDojo 🥥 DTU Mail 🖪 Completed 🦂 EDAM ontology br 📒 Listen 📙 Watch 🔹 📙 Other bookmarks
Elixir Bio. tools	13524 tools About Menu - jison 2 -
Update tool	Remove Validate Save
Summary* Function Labels	Links Download Documentation Publications Credits & Support Relations
JSON Permissions	
Basic information about the software You need to specify at least the name	e. e, homepage and a short description of the tool. See the Curation Guidelines 🗷.
Name 🕢 *	SignalP
Description 🛛 *	Prediction of the presence and location of signal peptide cleavage sites in amino acid sequences from different organisms.
Homepage URL 🕢 *	http://cbs.dtu.dk/services/SignalP/
Software version(s) 📀	4.1
	Add version

The editing interface provides some hints, and ensures that the information you set is in the right format. At any

moment, you can click on **Save** to save your edits, and immediately publish the changes online. The information you specified is checked to ensure it's in the right syntax. To (optionally) force a manual syntax check, click on **Validate**.

Important: The attributes required by *bio.tools* (tool name, description and homepage URL) are marked with a red asterix ^{*} in the editing interface, and must be given before an entry can be saved. Much more information is required

for the IFB catalogue, but this is not enforced by bio.tools !

Note: It's possible to create tool descriptions in JSON format directly in a text editor, and either paste these into the editing interface ("JSON" tab) or use the *bio.tools* API. For guidance on using the API, see the API Reference and the API Usage Guide.

Removing entries

To remove an entry, click on Update this record button (bottom right of the Tool Card). Then you can remove the

entry by clicking on

Remove

Warning: It shouldn't normally be necessary to remove a *bio.tools* entry, and you should try to avoid needing to do so! Although deleted entries are actually just hidden, not really deleted, removing an entry is definitive. There's no way back (other than emailing Registry Support).

6.1.3 3. Understand the information requirement

bio.tools

bio.tools requires only the name, description and homepage URL for a tool registration, but supports a comprehensive set of attributes for rich tool descriptions.

Note: The attributes supported by *bio.tools*, their structure and their syntax are defined in formalised XML schema called biotoolsSchema. You don't need to look at the schema, because everything is handled through *bio.tools*. If you'd like to learn more or contribute to this project, please head over to GitHub.

The IFB catalogue

The information requirement of the IFB catalogue is more demanding than *bio.tools*, and depends upon the type of tool (command-line tool, database *etc.*) that is being registered. A given tool attribute is *Mandatory*, *Recommended* or *Optional* for a given type of tool:

- Mandatory attributes MUST be specified.
- **Recommended** attributes **SHOULD** be specified, but are not strictly required.
- Optional attributes CAN be specified, to produce a rich tool description.

	Bioinformatics portal	Database portal	Web application	Desktop application	Command-line tool
Name					
Description					
Homepage					
Unique ID					
Tool type					
Scientific topics					
Scientific operations	0				
Type of input & output data	-		●	●	
Supported data formats	-	0	0	0	•
Primary publication					
Citation instructions	•	●	•	•	•
Credited developer	●	●	●	●	●
Credited maintainer	•	●	•	•	•
Credited institute	●	●	●	●	●
Credited funding agency	●	●	●	●	•
Maturity	●	●	●	●	●
5 Accessibility	•	Chapter 6.	Communi	ty-spēcific	guidēlines
Cost					

The above diagram is intended to give a quick overview of the information requirement. Only the main types of tool and most important attributes are shown. The *guidelines* below cover exactly what's needed for each type of tool, and go through the curation process in a step-by-step way.

Important: All tools in the IFB catalogue **must** have at least a minimal description, *i.e.* all *mandatory* attributes are specified. Tool providers are encouraged to provide an enhanced description which also includes all of the *recommended* attributes.

6.1.4 4. Plan your curation work

bio.tools entries

Important: Before you use *bio.tools* to create and edit tool descriptions, it's important to plan carefully the entries with respect to the types of tool and the functions they perform. Be sure to understand:

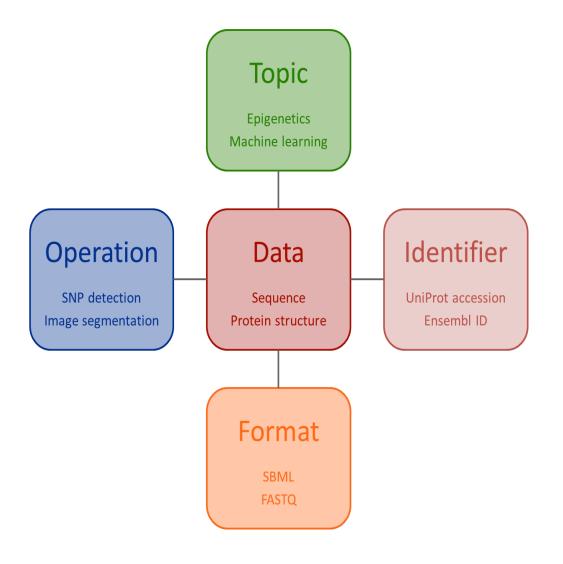
- 1. The type of tool being described this determines the information requirement and is covered in the section below on *tool type*.
- 2. The tool functionality and how it should be described covered in the section on *tool functions*.
- 3. Whether one or more entries are needed (see below).

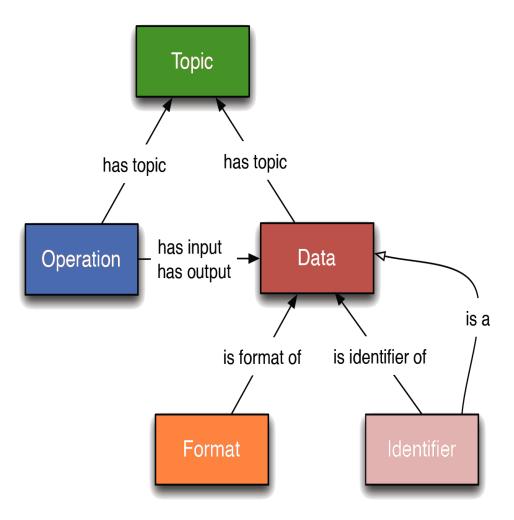
Plan what new entries (if any) are required to describe your tools:

- A discrete tool one which is clearly an individual, distinct entity should have it's own entry. This is the case for most *command-line tools* and *desktop applications*.
- *bio.tools* aims to catalogue *unique* tool functionality. Different implementations but with essentially the same functionality can be described by a single entry, *e.g.* a command-line tool that is later adapted into an R package for the Bioconductor suite, or which is served online via a Galaxy server.
- In some cases, *e.g.* complex software packages, it's not obvious whether to have one or multiple entries. Pick the option which mostly clearly illustrates the tool's functionality to end-users.
- Tool collections should be described by multiple entries. For example, one entry to describe a *suite*, and multiple other entries to describe the individual tools within that suite.
- Software with multiple interfaces should be described by a single entry, assuming these interfaces have essentially the same functionality. For example, a *command-line tool* whose functionality is also available via a *web application*, or a *database portal* with a *web API*.
- Many *database portals* provide the typical database functions (browse, deposit, search, visualise, analyse and download), often in different interface components. Usually one entry will suffice, but sometimes multiple entries are better, especially where the portal provides multiple analytical functions under different interfaces.
- For very complex entities such as *Bioinformatics portals*, do not try to describe everything in a single entry. Use a single entry for the portal, and multiple other entries for the things aggregated by the portal.

Familiarise yourself with EDAM

The EDAM ontology provides *bio.tools* with a controlled vocabulary to describe the scientific function of a tool, including the general scientific domain, specific operations it performs, types of input and output data, and supported data formats.





The EDAM ontology includes four main types of concept (or subontologies), shown in boxes above. The concepts are *Topic*, *Operation*, *Data* and *Format*, with *Identifier* being a specialisation of *Data*. Relationships between EDAM concepts are defined internally within the ontology. You don't need to worry about these details, as it's all handled by *bio.tools*.

Picking EDAM terms

Three EDAM browsers, each with different functionality, can be used to find EDAM terms:

- OLS
- BioPortal
- EDAM Browser

Tip: The EDAM term picker currently implemented in *bio.tools* is not very powerful. It's strongly recommended to use the browsers above. If you can't find exactly the terms you need, multiple searches using synonyms, alternative spellings *etc.* can help.

A much better term picker is on the way, and while not yet fully integrated into *bio.tools* is already very useful:

• EDAM Tool Annotator

You can use this to pick relevant topics and define the function of your tools. The ouput (in the bottom pane of the window) is a JSON object that can be copy-pasted into the *JSON* tab of the *bio.tools editing interface*, when editing a tool description.

If you can't find the right term, please request that it's added to EDAM via GitHub but first read the guidelines on how to request a term. It takes some time for new terms to be supported in *bio.tools*, so if you need many new terms, please plan ahead and contact the EDAM developers if you need help.

6.1.5 5. Describe your tools

The sections below match the tabs in the *bio.tools* editing interface.

Note: Only those tool attributes that are *Mandatory* or *Recommended* are described below, but you can of course also specify the *Optional* ones.

The {learn more} links take you to more detailed guidelines in the *bio.tools* Curators Guide. Follow these links whenever you're not sure about what information is needed.

Summary

In the *Summary* tab you specify basic information about the software:

Attribute	Requirement
Name	Mandatory
Description	Mandatory
Homepage URL	Mandatory

- **Name** is the short-form name by which the tool is commonly known, *e.g.* "BLAST" **not** "Basic Local Alignment Search Tool". Database names should follow a pattern where the name and abbreviation are given *e.g.* "The Protein Databank (PDB)" {learn more}.
- **Description** is a *concise* textual summary of the *tool function or purpose*. It can usually be copy-pasted from the tool homepage. Do not include statements about performance, provenance, governance *etc.* {learn more}.
- Homepage URL is the tool's homepage, or some URL that best serves this purpose {learn more}.

Important: A unique identifier - the *bio.tools* **toolID** - is created for a tool when a new entry is created. The ID value is a URL-safe version of the supplied tool name. The ID provides a persistent reference to the tool, used by *bio.tools* and other systems. toolIDs are used in the Tool Card URLs, which can be represented in a short form as a "compact URI" or "CURIE":

- toolID: signalp
- CURIE: biotools:signalp
- Tool Card URL: https://biotools/signalp

The ID should be sensible and intuitive. For databases, or tools with long names, the abbreviation should be used. For example, the GnpIS tool tool has the ID "gnpis" and *not* "Genetic and Genomic Information System".

Tip: The toolID is **not** currently editable, so if you want the ID to differ from the name (*e.g.* an ID of "PDB" for the tool name "Protein databank (PDB)", you have to apply a workaround:

- 1) create the entry giving a value for "Name" which is the desired ID value, e.g. "PDB"
- 2) Save the entry
- 3) Edit the entry, resetting the name, e.g. to "Protein Databank (PDB)"

To request an ID change post-registration (to be avoided!) you have to mail Registry Support.

Labels

In the *Labels* tab you specify miscellaneous scientific, technical and administrative details, expressed in terms from controlled vocabularies:

ATTRIBUTE	REQUIREMENT
Tool type	Mandatory
Торіс	Mandatory
Cost	Mandatory
License	Mandatory (Desktop application, Command-line tool)
Operating system	Mandatory (Desktop application)
	Recommended (Command-line tool)
Maturity	Recommended
Accessibility	Recommended (Bioinformatics portal, Database portal, Web application)
Language	Recommended (Command-line tool)

- Tool type describes the type of the tool: a *bio.tools* entry can have more than one type. See *below* {learn more}.
- **Topic** is the general scientific domain the tool serves, or other general category (an EDAM term). See *below* {learn more}.
- **Cost** is the monetary cost of acquiring the software {learn more}.
- License is a software or data usage license. See *below* {learn more}.
- **Operating system** is the operating system supported by a downloadable software package pick all that apply {learn more}.
- **Maturity** is how mature the software product is; *Emerging*, *Mature* or *Legacy*. Don't pick *Mature* for tools which aren't really mature yet! {learn more}.
- Accessibility is whether there are non-monetary restrictions on accessing an online service; *Open access, Open access (with restrictions)* or *Restricted access.* Read the definitions before picking these terms! {learn more}.
- Language is the name of a programming language the tool source code was written in {learn more}.

Tip: You can use **Collection** to assign tools which are somehow related to one or more groups. These collections can have any names you like. Other ways to group tools are by creating a *bio.tools* subdomain (from *Menu...Manage subdomains*) and by defining relations between tools.

Note: ELIXIRNode and ELIXIRPlatform define the name of an ELIXIR node or ELIXIR platform, respectively, that is credited for the tool. All tools in the IFB catalogue will have the ELIXIRNode credit set to "France". These are not normally be set by *bio.tools* users {learn more}. ELXIRCommunity defines a community (ELIXIR or otherwise) to which the resource is directly relevant - you can select as many as you wish.

Tool type

The scope of *bio.tools* is very broad - ranging from simple scripts to comprehensive bioinformatics portals - as defined by 15 different tool types. The vast majority of entries are of the following types:

TYPE	DESCRIPTION
Bioinformatics	A web site providing a platform/portal to multiple resources used for research in a focused
portal	area, including biological databases, web applications, training resources and so on.
Database portal	A Web site providing a portal to a biological database, typically allowing a user to browse,
	deposit, search, visualise, analyse or download data.
Web application	A tool with a graphical user interface that runs in your Web browser.
Desktop applica-	A tool with a graphical user interface that runs on your desktop environment, e.g. on a PC
tion	or mobile device.
Command-line	A tool with a text-based (command-line) interface.
tool	

Other common types incude:

TYPE	DESCRIPTION
Web API	An application programming interface (API) consisting of endpoints to a request-response
	message system accessible via HTTP. Includes everything from simple data-access URLs
	to RESTful APIs.
Workflow	A set of tools which have been composed together into a pipeline of some sort. Such
	tools are (typically) standalone, but are composed for convenience, for instance for batch
	execution via some workflow engine or script.
Suite	A collection of tools which are bundled together into a convenient toolkit. Such tools typ-
	ically share related functionality, a common user interface and can exchange data conve-
	niently. This includes collections of stand-alone command-line tools, or Web applications
	within a common portal.
Workbench	An application or suite with a graphical user interface, providing an integrated environment
	for data analysis which includes or may be extended with any number of functions or tools.
	Includes workflow systems, platforms, frameworks etc.
Workflow	A set of tools which have been composed together into a pipeline of some sort. Such
	tools are (typically) standalone, but are composed for convenience, for instance for batch
	execution via some workflow engine or script.
Library	A collection of components that are used to construct other tools. bio.tools scope includes
	component libraries performing high-level bioinformatics functions but excludes lower-
	level programming libraries.

A single *bio.tools* entry is annotated with one or more types, reflecting different facets of the tool described by the entry. Be sure to understand the type(s) of tool you have, because it determines the information that's expected. A few suggestions:

- *Bioinformatics portals* aggregate information about tools and databases, but don't (typically) directly serve them. Only use *Bioinformatics portal* for sites that cover multiple other resources, each which are their own distinct entity (and should have their own *bio.tools* entries). Good examples include IMGT and wheatIS.
- *Suite* might be more applicable than *Bioinformatics portal*. Example include Web application suites such as CRISRP-Cas++ and EvryRNA, and suites of command-line tools such as BioConductor.
- *Workbench* might be also be more applicable than *Bioinformatics portal*. This includes online and desktop integrated environements. Example include the general-purpose Galaxy workbench and domain-specific ones such as MetExplore and MicroScope.

- Typically use only one of *Bioinformatics portal*, *Database portal* or *Web application* in a single entry. If the resource is providing a database, then just go with *Database portal*, a good example being Norine.
- In general, often a singe tool type will do. For example, LoRDEC (a *Command-line tool*), GINsim (a *Desktop application*), and Ocean Gene Atlas or Genomicus (both are *Web application*).
- But do pick all the types that apply. For example the BOOSTER *Command-line tool* is also available as a *Web application* (and if these implementations have essentially the same functionality, they'd be described in a single *bio.tools* entry).
- If a database has an API (most do!) then use both Database portal and Web API, for example aNISEED.
- Use the more specialised tool types where they are applicable, for example *Workflow* for Workflow for Workflow4 Metabolomics and *Library* for any R pacages.

Tip: Software is complex and it can be tricky to assign a type. Make sure you understand the tool type definitions before you use them. For example, in *bio.tools* a *Web service* is specifically a SOAP+WSDL implementation. Most likely you need *Web API* (which covers most APIs nowadays) or just *Web application* (for a tool delivered via the Web but without an API).

License

All downloadable software should be licensed. If you can't find your license in the list, use one of the terms below:

Note: There are many good reasons why you should license your software, ideally picking a FOSS (Free and Open Source Software) license. Read A Quick Guide to Software Licensing for the Scientist-Programmer. Some types of tools *e.g.* *Web application" are not licensed, but instead, should have a *Terms of use* document. Proprietary licenses are definitely not open-source or, and should be avoided!

If your sofware is available under a license not supported by *bio.tools*, then please request the license is added. If you find yourself picking **Not licensed** - this is bad - license your software!

Topic

Topic is the place to tag your tool with EDAM terms describing the scientific domain the tool serves, or other general category.

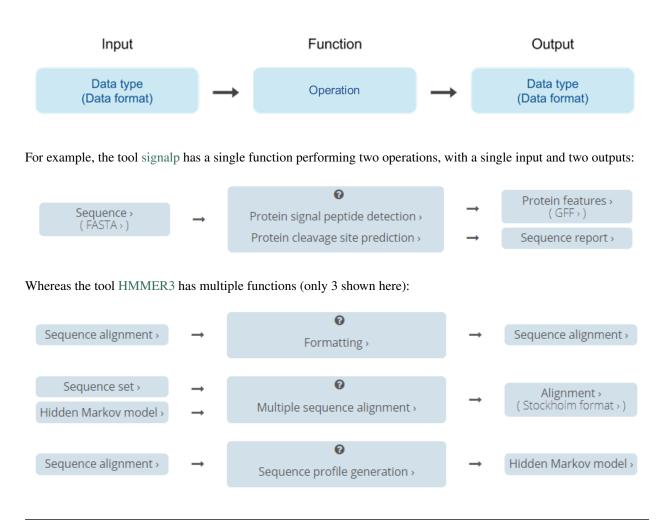
- specify the most important and relevant scientific topic; up to 3 topics will usually suffice
- don't exhaustively specify all the topics of lower or secondary relevance

Tip: Don't rely on the term picker included in *bio.tools* to find topics and other EDAM terms - use the *EDAM browsers* or EDAM Tool Annotator instead. They are much more powerful!

Function

In the *bio.tools* software model, a tool has one or more basic functions, or modes of operation. Each **function** performs at least one **operation**, and has one or more primary **inputs** and **outputs**. Each input and output are of single defined **type of data** and list one or more supported **format**(s).

This is shown in a diagram on the Tool Cards that look like this:



Note: The HMMER3 entry has very nicely annotated functionality, but is a good example of where the entry would be easier to understand if the functionality was described in separate entries - retaining the existing entry for the suite, but creating a new entry for each of the HMMER programs (alimask, hmmalign, hmmbuid *etc.*).

In the Function tab you specify the functions of the tool, expressed in concepts from the EDAM ontology.

ATTRIBUTE	REQUIREMENT
Operation	Mandatory (Database portal, Web application, Desktop application, Command-line tool)
Input->data	Mandatory (Command-line tool)
	Recommended (Web application, Desktop application)
Input->format	Recommended (Command-line tool)
Output->data	Mandatory (Database portal, Command-line tool)
	Recommended (Web application, Desktop application)
Output->format	Recommended (Command-line tool)

- **Operation** describes the basic operation(s) performed by this software function. See *below* {learn more}.
- Data is a type of primary input or output data. See *below* {learn more}.
- Format is the allowed format(s) of the input or output data. See *below* {learn more}.

Note: You can use Note to add a concise comment about this function, if this is not apparent from the software

description and EDAM annotations.

Tip: When deciding how to describe your tools, in terms of *bio.tools* entries, their functions and operations, always keep the end-user in mind and try to describe your tools in a way that will be clear to them.

It can be difficult to find the right terms to describe a tools operation(s), input(s) or output(s). It's highly recommended to use EDAM Tool Annotator to describe the function, and carefully copy-paste the JSON ouput (in the bottom pane of the window) into the *JSON* tab of the *bio.tools editing interface*. Or use the OLS, BioPortal or EDAM Browser alongside *bio.tools* when describing your tools. If you're not sure, mail registry-support for help.

Operation

Before describing your tools, you should carefully identify the distinct functions and the individual operations associated with each one. This is often straighforward, as different functions (modes) typically perform distinct operations:

- if a tool has an option between doing one thing or another, then you should annotate the operations as distinct functions
- if in contrast a tool always does one or more things, then you should annotate these as distinct operations within a single function
- only specify the primary functions and operations, from a typical end-user perspective tools often do many other things than its central, advertised purpose you don't need to describe everything!

Tip: Database portal usually provide one ore more of a common set of operations:

- Browse no term in EDAM yet
- Deposit Deposition (http://edamontology.org/operation_3431)
- Search Database search (http://edamontology.org/operation_2421)
- Visualise Visualisation (http://edamontology.org/operation_0337)
- Analyse Analysis (http://edamontology.org/operation_2945)
- Download Data retrieval (http://edamontology.org/operation_2422)

When annotating the operations, you should specify all of these that apply. Consider carefully whether the *Analyis* operation(s) would be better listed as functions of discrete tools described in their own own entries (see *bio.tools entries*).

Data

- data terms must be correctly associated with the operation(s)
- only specify the primary inputs and outputs, *e.g.* a sequence alignment tool would be annotated as reading sequences (input), and writing a sequence alignment (output), but not with gap insertion and extension penalties, or other parameters.

Tip: For *Database portal*:

• for *Deposition* and *Data retrieval* operations, you can associate the types of *data* available for upload (input) or download (output).

• for *Search* operation, you can specify *Database search results* (http://edamontology.org/data_2080) as an output, or some other more specific term in the EDAM Data subontology.

Format

- format terms must be correctly associated with an input or output data type
- specify the most widely used of the supported data formats it can be impractical / onerous to be exhaustive!

Links

In the *Links* tab you specify miscellaneous links for the tool. The type of information obtained when resolving the link is specified by *Link type*:

ATTRIBUTE	REQUIREMENT
Repository	Recommended (Desktop application, Command-line tool)
Mailing list	Recommended
Issue tracker	Recommended (Database portal, Web application, Desktop application, Command-line
	tool)
Helpdesk	Recommended (Database portal)

- Repository is where source code, data and other files may be downloaded, e.g. a GitHub repo, or an FTP site.
- Mailing list is for software announcements, discussions, support etc.
- Issue tracker is for software issues, bug reports, feature requests etc.
- Helpdesk is a phone line, web site or email-based system providing help to the end-user of the software.

Tip: A single link might resolve to a page containing information of more than one type; in these cases pick all of the types that apply!

Note: It's strongly recommended to put your source code and other downloadable resources in a public repository such as GitHub. It takes little effort to do so. A repo can serve as a homepage for your tool, and provide an issue tracker and open forum for discussion. If you don't have a repo, you should at least provide a *downloads page*.

Caution: Currently, to assign a link to more than one type you have to enter the URL more than once, picking a different type each type. In future, you'll be able to enter the URL once and pick multiple types.

Download

In the Download tab you specify links to downloads for your software.

TYPE	REQUIREMENT	
Source code	Recommended (Database portal, Web application, Desktop application, Command-line	
	tool)	
Binaries	Recommended (Desktop application, Command-line tool)	
Software package	Recommended (Desktop application, Command-line tool)	
Downloads page	Recommended (Database portal, Desktop application)	
API specification	Recommended (Database portal - with API)	
Test data	Recommended (Desktop application, Command-line tool)	
Test script	Recommended (Command-line tool)	

- Source code should trigger a download of the *latest* source code available (typically the latest stable version)
- Binaries should trigger a download of the latest binaries available
- **Software package** should trigger a download of the *latest* software package.
- Downloads page is a Web page summarising general downloads available for the software.
- **API specification** is a file providing a machine-readable API specification for the software, *e.g.* Swag-ger/OpenAPI, WSDL or RAML file. It's *not* for human-readable API documentation (see *documentation* for that).
- Test data is data for testing the software is working correctly.
- **Test script** is a script used for testing testing whether the software is working correctly.

Tip: With the exception of **Downloads page**, the expectation is that a link annotated in the *Download* section will trigger a download of a file. If you're adding a link which doesn't have this behaviour, you should see whether an attribute in the *Links* section is more appropriate.

Note: Command-line specification and API specification are files providing a machine-readable specification of the command line or API, for the software. These are *not* used for the typical human-readable documentation (see *Documentation* for that).

Documentation

In the *Documentation* tab you link to documentation about the software:

TYPE	REQUIREMENT		
General	Mandatory (Database portal, Web application, Desktop application, Command-line tool)		
API documenta-	Mandatory (Database portal or Web application - with API)		
tion			
Terms of use	Mandatory (Bioinformatics portal, Database portal, Web application)		
Command-line op-	Mandatory (Command-line tool)		
tions			
Citation instruc-	Recommended		
tions			
Contributions pol-	Recommended		
icy			
Training material	Recommended		
Installation in-	Recommended (Desktop application, Command-line tool)		
structions			
User manual	Recommended (Desktop application)		
Release notes	Recommended (Desktop application, Command-line tool)		

- **General** is for general documentation. If your tool doesn't have a dedicated documentation page, but is documented elsewhere (*e.g.* on the homepage or a GitHub README.md) then specify that URL instead.
- **API documentation** is human-readable API documentation, and should be specified for any *Database portal* or *Web application* with an API.
- Terms of use are rules that one must agree to abide by in order to use a service. Note, this is different to License!
- Command-line options are human-readable documentation about the command-line interface of a tool.
- **Citation instructions** give information on how to correctly cite use of the software; typically which publication(s) to cite, or something more general, e.g. a form of words to use. This is especially important where there are multiple relevant *publications*.
- Contributions policy is information about policy for making contributions to the software project.
- Training material is an online training material such as a tutorial, a presentation, video etc.
- Installation instructions are instructions how to install the software.
- User manual is information on how to use the software, structured into a comprehensive user manual (don't just link here to general documentation).
- **Release notes** are notes about a software release or changes to the software (a change log). For example a CHANGELOG.md file on GitHub.

Note: You should create **contribution guidelines** to communicate how people should contribute to your open source project. In GitHub this is done by createing a CONTRIBUTING.MD file. Lots of good advice, templates and examples are available (*e.g.* Atom editor, Ruby on Rails and Open Government).

A well maintained **change log** will make it easier for users and contributors to see precisely what notable changes have been made between each release (or version) of the project. For some great advice, see keepachangelog.com.

Note: Command-line tools should always have a human-readable description of their **command-line options**. Similarly, an API on a *Database portal* or *Web application* should have a human-readable description of their API. If machine-readable command-line or API specifications (files) are also available, then you should link to those in the *Download* section.

Important: You must not specify a link to a general page where a more specific one is available. For example, don't link to the homepage in the **General** field if, in fact, there's a dedicated page for documentation. If you want to link to some documentation not of a type supported by biotoolsSchema, then use the **Other** value.

Caution: Currently, to assign a documentation to more than one type you have to enter the URL more than once, picking a different type each type. In future, you'll be able to enter the URL once and pick multiple types.

Publications

In the *Publications* tab you specify publications about the software:

ATTRIBUTE	REQUIREMENT
Primary publica-	Mandatory
tion	

Publications are defined as one of the following types:

TYPE	DESCRIPTION	
Primary	The principal publication about the tool itself; the article to cite when ac-	
	knowledging use of the tool.	
Method	A publication describing a scientific method or algorithm implemented by	
	the tool.	
Usage	A publication describing the application of the tool to scientific research, a	
	particular task or dataset.	
Benchmarking study	A publication which assessed the performance of the tool.	
Review	A publication where the tool was reviewed.	
Other	A publication of relevance to the tool but not fitting the other categories.	

and can have the following attributes defined:

Attribute	Description	
pmcid	PubMed Central Identifier of a publication about the software.	
pmid	PubMed Identifier.	
doi	Digital Object Identifier.	
note	Comment about the publication.	
version	Version information (typically a version number) of the software applicable	
	to this publication.	

• Specify at least the primary publication for your tool, and ideally any others that are relevant.

• Pick one or more types for each publication, as applicable.

Tip: You should specify **DOI** for publications (if available) and do not have to also specify **pmid** and **pmcid**. But if you do, then be sure to specify multiple IDs for a single publication within a single publication group.

You can ignore **note** and **version**.

Note: It's very important that your tool has some form of publication, if for no other reason than to make it citable. If you don't have a publication in the scientific press, then you can use Zenodo to create a DOI for this purpose. Such a DOI should resolve to a page describing the tool. For example http://doi.org/10.5281/zenodo.3519603.

Caution: Currently, to assign a publicaton to more than one type you have to enter the DOI more than once, picking a different type each type. In future, you'll be able to enter the DOI once and pick multiple types.

Credits & Support

In the *Credits & Support* tab you specify individuals or organisations that should be credited, or may be contacted about the software. Credits include all type of entities that contributed to the development, maintenance or provision of the resource:

ATTRIBUTE	REQUIREMENT
Primary contact	Mandatory
Credited institute	Recommended
Credited funding	Recommended
agency	
Credited developer	Recommended
Credited main-	Recommended
tainer	

Creditable entities have one of the following types:

TYPE	DESCRIPTION
Person	Credit of an individual.
Project	Credit of a community software project not formally associated with any single institute.
Division	Credit of or a formal part of an institutional organisation, e.g. a department, research group,
	team, etc
Institute	Credit of an organisation such as a university, hospital, research institute, service center,
	unit etc.
Consortium	Credit of an association of two or more institutes or other legal entities which have joined
	forces for some common purpose. Includes Research Infrastructures (RIs) such as ELIXIR,
	parts of an RI such as an ELIXIR node etc.
Funding agency	Credit of a legal entity providing funding for development of the software or provision of
	an online service.

and also have a role:

ROLE	DESCRIPTION	
Developer	Author of the original software source code.	
Maintainer	Maintainer of a mature software providing packaging, patching, distribution etc.	
Provider	Institutional provider of an online service.	
Documentor	Author of software documentation including making edits to a bio.tools entry.	
Contributor	Some other role in software production or service delivery including design, deployment,	
	system administration, evaluation, testing, documentation, training, user support etc.	
Support	Provider of support in using the software.	
Primary contact	The primary point of contact for the software.	

You must specify at least:

• A credit of role **Primary contact** with an applicable type. You can opt to give more than one primary contact, for example specifing one for a project and another for a person.

It's recommended to specify:

- A credit of type **Institute** with one ore more applicable roles
- A credit of type **Funding agency**
- A credit of role **Developer** with one ore more applicable types
- A credit of role Maintainer with one ore more applicable types

For any credit, you can specify any of the following:

Attribute	Description
name	Name of the entity that is credited.
orcidid	Unique identifier (ORCID iD) of a person that is credited.
gridid	Unique identifier (GRID ID) of an organisation that is credited.
rorid	Unique identifier (ROR ID) of an organisation that is credited.
fundrefid	Unique identifier (FundRef ID or Funder ID) of a funding organisation that is credited.
email	Email address.
url	URL, e.g. homepage of an institute.
tel	Telephone number.
typeEntity	Type of entity that is credited (see above)
typeRole	Role performed by entity that is credited (see above)
note	A comment about the credit.

Important: A credit can have multipe **role**. When creating a credit, pick all of the roles that apply; don't create duplicate credit groupings!

Note: It's strongly recommended that if you (or other people to be credited) don't have an ORCID iD, that you get one now. ORCID provides a persistent digital identifier that distinguishes you from every other researcher and, through integration in key research workflows such as manuscript and grant submission, supports automated linkages between you and your professional activities ensuring that your work is recognized.

Note: Nearly all organisations credited in *bio.tools* will have a GRID ID. The Global Research Identifier Database (GRID) provides unambiguous institutional information at persistent IDs, to ensure data consistency.

Relations

In the *Relations* tab you can specify details of a relationship this software shares with other software registered in *bio.tools*.

The relationships currently available:

Relation	Description	
isNewVersionOf	The software is a new version of an existing software, typically providing	
	new or improved functionality.	
hasNewVersion	(inverse of above)	
uses	The software provides an interface to or in some other way uses the func-	
	tions of other software under the hood, e.g. invoking a command-line tool	
	or calling a Web API, Web service or SPARQL endpoint to perform its	
	function.	
usedBy	(inverse of above)	
includes	A workbench, toolkit or workflow includes some other, independently avail-	
	able, software.	
includedIn	(inverse of above)	

You can ignore this for now, except:

- when annotating a Suite (or other collection) it's recommended to specify other tools that the suite includes
- when annotating a Workflow it's recommended to specify other tools that the workflow uses

JSON

In the *JSON* tab you see all the information that you've specified for a tool so far. You can work directly in this pane if you wish. This can be very useful when using the EDAM Tool Annotator to define the tool's function (see the section on *EDAM*.)

Permissions

In the *Permissions* tab you can decide to make the entry either editable only by yourself, a list of users or anyone. See the section on *bio.tools accounts*.

6.2 Workflow composition (Lorentz workshop)

These instructions provide a quick guide to the steps to register your tools in bio.tools and describe them using the EDAM ontology to a standard suitable for applications in workflow composition. They were written to support the workshop Automated Workflow Composition in the Life Sciences hosted by the Lorentz Center.

Help is available:

- To get help using *bio.tools*, or for general curation advice, please mail registry-support.
- To get help using the EDAM ontology, please head over to <GitHub 'https://github.com/edamontology/edamontology>'_ and post an issue.
- If you have questions specifically about curation of tools for the Lorent workshop, you can mail Jon Ison directly.

Note: For more information and help, see:

- Guidelines for IFB tools cover similar ground to this document, but in more detail.
- The bio.tools Curators Guide provides in-depth curation guidelines.
- The biotoolsSchema documentation summarises the attributes, information model and controlled vocabularies including the EDAM ontology used by *bio.tools*.

• The EDAM ontology documentation everything you need to know about contributing to, editing and developing EDAM.

If you find a bug in this document, or have any questions or suggestions, please post them on GitHub.

6.2.1 1. Get a bio.tools account

You'll need an account to create *bio.tools* entries or edit existing ones. Creating an account is simple: just go to Sign-up

bio.tools and click on at the top-right corner of the page.

You'll be asked for a username, email address and password. Your account will be setup immediately.

Note: *bio.tools* entries are owned by the individuals who created them. Owners may grant edit rights, or transfer ownership of their entries to other registered users - these rights are set in the *Permissions* tab of the *bio.tools* editing interface.

The rightful owner of a *bio.tools* entry is usually the person who developed the tool, or provides an online service, but it can be some other responsible person, *e.g.* a dedicated curator.

6.2.2 2. Claim your bio.tools entries

As a software developer or service provider, you should own the *bio.tools* entries describing your tools, by claiming ownership of existing entries or creating new ones. Alternatively, if you just want to edit a tool description, than you can request edit rights for it.

You'll need to login first, by clicking on



at the top-right corner of the page.

To see whether a tool is already registered, search for it by its name. Simply type the name in the search box. You may need to click on the *Name* facet to narrow-down the search:

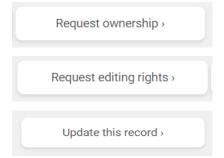
Apps ★ Bookmarks 🔇	Journal access 🍯 Mail – EFoster@swa 🐔 ClassDojo 🥥 DTU Mail 🛐 Completed	 Q ☆ I I I I I I I I I I I I I I I I I I I
	ignal	13524 tools About Login Sign-up
Sort by Update	Everything Topic Operation Input Output Tool type Langua Accessibility Cost License Credit Collection <u>Name</u>	ige I Display as Compact Detailed
	signalAlign	
Ocean Gene Atla:	Atlas of Cancer Signalling Network (ACSN)	
The Ocean Gene A	MetaboSignal	c gene sequence catalogs (ENA), sample environmental
context (PANGAEA	LnSignal	reads onto gene catalogs). User queries are composed
of either a sequence catalogs are identif		nce alignment. Homologs of the user query in the gene their read based estimated abundance are displayed in
interactive maps ar	bam signal s	hin its context of marine environmental homologs as well
as known homolog	Signal-CF	
	Signal-3L	
Ecology Marin	eSIGNAL	
Phylogenetic tree	SignalP	alignment Quantification Map drawing
Sequence alignmen	t i	

Once you find your entry you can go ahead and update it. If you can't find the entry, you'll need to create it.

Important: Many of the tools you need already have been registered, but possibly with only very basic details. You will need to take ownerhsip or request edit rights on these entries to improve them. Before starting work, please ensure you understand the *information requirement* and follow the *guidelines* below.

Updating entries

To edit an existing entry, you need to click through to the Tool Card for the tool in question, *e.g.* https://bio.tools/ signalp. You'll see a one or two buttons at the bottom right of the Tool Card, depending on whether you're logged in, and own the entry or not.

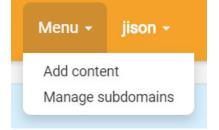


- Click on Request ownership if you want to claim ownership of the entry
- Click on Request editing rights if you want to edit rights on the entry, but not own it
- Click on Update this record to edit the entry (visible only if you own the entry or have editing rights)

Note: It can take a little while for other users to respond to requests for edit rights or ownership. If these are not granted within a day or two, please mail registry-support.

Creating entries

To create new entries you'll need to be logged onto *bio.tools*. Click on *Menu* ... Add content:



bio.tools editing interface

The *bio.tools* editing interface helps you to create valid tool descriptions. It's organised into different tabs (*Summary*, *Function*, *Labels etc.*):

😵 bio.tools x +		- 🗆 ×
← → C △	् 🖈 🔟 🕲 🖉 🦉	🛐 🕝 🤷 🚥 🔜 🌄 🍖 🔂 🍎 🗄 ten 📙 Watch 🔹 📄 📴 Other bookmarks
Elixir bio.tools	13524 tools About	Menu - jison 2 -
Update tool		Remove Validate Save
Summary + Function Labels JSON Permissions	Links Download Documentation Publications (Credits & Support Relations
Basic information about the software You need to specify at least the name	, homepage and a short description of the tool. See the Curation Guid	Jelines 🗗
Name 🕢 *	SignalP	
Description 🛛 *	Prediction of the presence and location of signal peptide cleavage site amino acid sequences from different organisms.	is in
Homepage URL 😪 *	http://cbs.dtu.dk/services/SignalP/	
Software version(s) 🕢	4.1	×
	Add version	

The editing interface provides some hints, and ensures that the information you set is in the right format. At any

moment, you can click on **Save** to save your edits, and immediately publish the changes online. The information you specified is checked to ensure it's in the right syntax. To (optionally) force a manual syntax check,

click on

Validate

Important: The attributes required by bio.tools (tool name, description and homepage URL) are marked with a red

asterix * in the editing interface, and must be given before an entry can be saved. You will need to provide more information to support workflow composition - especially about the tool *function* - but this is not enforced by *bio.tools* !

Note: It's possible to create tool descriptions in JSON format directly in a text editor and paste these into the editing interface ("JSON" tab), where you see all the information that you've specified for a tool so far. You can work directly in this pane if you wish. This can be very useful when using the EDAM Tool Annotator to define the tool's function (see the section on *EDAM*.)

Removing entries

To remove an entry, click on Update this record button (bottom right of the Tool Card). Then you can remove the

entry by clicking on

Remove

Warning: It shouldn't normally be necessary to remove a *bio.tools* entry, and you should try to avoid needing to do so! Although deleted entries are actually just hidden, not really deleted, removing an entry is definitive. There's no way back (other than emailing Registry Support).

6.2.3 3. Plan your curation work

Information requirement

bio.tools requires only the name, description and homepage URL for a tool registration, but supports a comprehensive set of attributes for rich tool descriptions.

To support workflow composition, very careful curation of tool functionality - it's input(s), operation(s) and output(s) - is required. The *guidelines* below cover exactly what's needed, and go through the curation process in a step-by-step way.

Note: The attributes supported by *bio.tools*, their structure and their syntax are defined in formalised XML schema called biotoolsSchema. You don't need to look at the schema, because everything is handled through *bio.tools*. If you'd like to learn more or contribute to this project, please head over to GitHub.

Before you start

Important: Before you use *bio.tools* to create and edit tool descriptions, be sure to understand:

- 1. The type of tool being described covered below in the section below on *Basic information*.
- 2. The tool functionality and how it should be described covered in the section on *tool functions*.
- 3. Whether one or more entries are needed (see below).

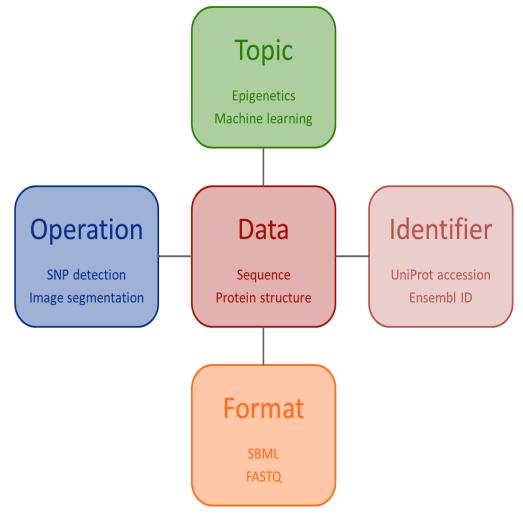
Plan what new entries (if any) are required to describe your tools:

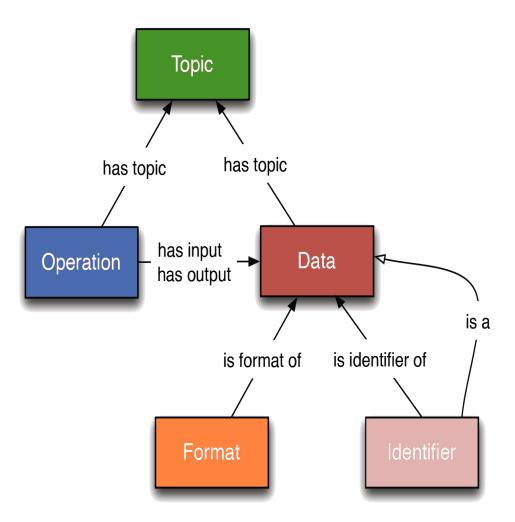
- A discrete tool one which is clearly an individual, distinct entity should have it's own entry. This is the case for most *command-line tools* and *desktop applications*.
- *bio.tools* aims to catalogue *unique* tool functionality. Different implementations but with essentially the same functionality can be described by a single entry, *e.g.* a command-line tool that is later adapted into an R package for the Bioconductor suite, or which is served online via a Galaxy server.
- In some cases, *e.g.* complex software packages, it's not obvious whether to have one or multiple entries. Pick the option which mostly clearly illustrates the tool's functionality to end-users.
- Tool collections should be described by multiple entries. For example, one entry to describe a *suite*, and multple other entries to describe the individual tools within that suite.
- Software with multiple interfaces should be described by a single entry, assuming these interfaces have essentially the same functionality. For example, a *command-line tool* whose functionality is also available via a *web application*, or a *database portal* with a *web API*.

For more information, see the IFB tools tutorial.

Familiarise yourself with EDAM

The EDAM ontology provides *bio.tools* with a controlled vocabulary to describe the scientific function of a tool, including the general scientific domain, specific operations it performs, types of input and output data, and supported data formats.





The EDAM ontology includes four main types of concept (or subontologies), shown in boxes above. The concepts are *Topic*, *Operation*, *Data* and *Format*, with *Identifier* being a specialisation of *Data*. Relationships between EDAM concepts are defined internally within the ontology. You don't need to worry about these details, as it's all handled by *bio.tools*.

Picking EDAM terms

Three EDAM browsers, each with different functionality, can be used to find EDAM terms:

- OLS
- BioPortal
- EDAM Browser

Tip: The EDAM term picker currently implemented in *bio.tools* is not very powerful. It's strongly recommended to use the browsers above. If you can't find exactly the terms you need, multiple searches using synonyms, alternative spellings *etc.* can help.

A much better term picker is on the way, and while not yet fully integrated into *bio.tools* is already very useful:

• EDAM Tool Annotator

You can use this to pick relevant topics and define the function of your tools. The ouput (in the bottom pane of the window) is a JSON object that can be copy-pasted into the *JSON* tab of the *bio.tools editing interface*, when editing a tool description.

If you can't find the right term, please request that it's added to EDAM via GitHub but first read the guidelines on how to request a term. It takes some time for new terms to be supported in *bio.tools*, so if you need many new terms, please plan ahead and contact the EDAM developers if you need help.

6.2.4 4. Describe your tools

Note: Only those tool attributes that are *Mandatory* in *bio.tools*, or which are required to support workflow composition are described below, but you can of course specify much mre. The {learn more} links take you to more detailed guidelines in *IFB tools* or the *bio.tools* Curators Guide. Follow these links whenever you're not sure about what information is needed.

Basic information

In the Summary tab you specify basic information about the software:

- Name is the short-form name by which the tool is commonly known, *e.g.* "BLAST" not "Basic Local Alignment Search Tool". Database names should follow a pattern where the name and abbreviation are given *e.g.* "The Protein Databank (PDB)" {learn more}.
- **Description** is a *concise* textual summary of the *tool function or purpose*. It can usually be copy-pasted from the tool homepage. Do not include statements about performance, provenance, governance *etc.* {learn more}.
- Homepage URL is the tool's homepage, or some URL that best serves this purpose {learn more}.

Important: A unique identifier - the *bio.tools* **toolID** - is created for a tool when a new entry is created. The ID value is a URL-safe version of the supplied tool name. The ID provides a persistent reference to the tool, used by *bio.tools* and other systems. toolIDs are used in the Tool Card URLs, which can be represented in a short form as a "compact URI" or "CURIE":

- toolID: signalp
- **CURIE:** *biotools:signalp*
- Tool Card URL: https://biotools/signalp

The ID should be sensible and intuitive. For databases, or tools with long names, the abbreviation should be used. For example, the GnpIS tool tool has the ID "gnpis" and *not* "Genetic and Genomic Information System".

Tip: The tooIID is **not** currently editable, so if you want the ID to differ from the name (*e.g.* an ID of "PDB" for the tool name "Protein databank (PDB)", you have to apply a workaround:

- 1) create the entry giving a value for "Name" which is the desired ID value, e.g. "PDB"
- 2) Save the entry
- 3) Edit the entry, resetting the name, e.g. to "Protein Databank (PDB)"

To request an ID change post-registration (to be avoided!) you have to mail Registry Support.

In the *Labels* tab you specify miscellaneous scientific, technical and administrative details, expressed in terms from controlled vocabularies. For now, annotate the following:

- **Tool type** is where you specify the type(s) of software that is described by the entry. A single *bio.tools* entry may be annotated with one or more types, reflecting different facets of the tool described by the entry. {learn more}.
- **Topic** is the place to tag your tool with EDAM terms describing the scientific domain the tool serves, or other general category.
 - specify the most important and relevant scientific topic; up to 3 topics will usually suffice
 - don't exhaustively specify all the topics of lower or secondary relevance

Note: The scope of *bio.tools* is very broad - ranging from simple scripts to comprehensive bioinformatics portals - as defined by 15 different tool types. The vast majority of tools used to compose workflows are of the following types:

TYPE	DESCRIPTION
Command-line	A tool with a text-based (command-line) interface.
tool	
Web application	A tool with a graphical user interface that runs in your Web browser.
Desktop applica-	A tool with a graphical user interface that runs on your desktop environment, e.g. on a PC
tion	or mobile device.
Web API	An application programming interface (API) consisting of endpoints to a request-response message system accessible via HTTP. Includes everything from simple data-access URLs to RESTful APIs.

Tip: Don't rely on the term picker included in *bio.tools* to find topics and other EDAM terms - use the *EDAM browsers* or EDAM Tool Annotator instead. They are much more powerful!

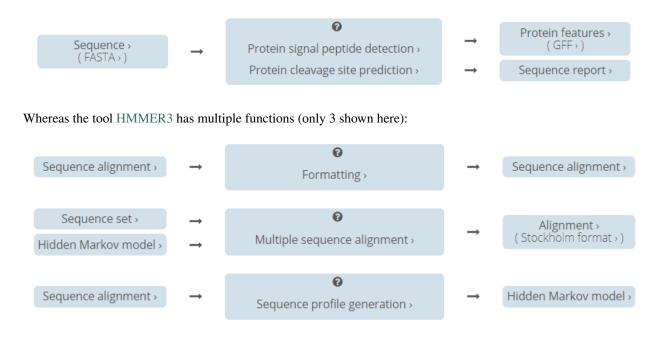
Function

In the *bio.tools* software model (biotoolsSchema), a tool has one or more basic functions, or modes of operation. Each **function** performs at least one **operation**, and has one or more primary **inputs** and **outputs**. Each input and output are of single defined **type of data** and list one or more supported **format**(s).

This is shown in a diagram on the Tool Cards that look like this:



For example, the tool signalp has a single function performing two operations, with a single input and two outputs:



Note: The HMMER3 entry has very nicely annotated functionality, but is a good example of where the entry would be easier to understand if the functionality was described in separate entries - retaining the existing entry for the suite, but creating a new entry for each of the HMMER programs (alimask, hmmalign, hmmbuid *etc.*).

In the Function tab you specify the functions of the tool, expressed in concepts from the EDAM ontology.

- **Operation** describes the basic operation(s) performed by this software function. See *below* {learn more}.
- Data is a type of primary input or output data. See *below* {learn more}.
- Format is the allowed format(s) of the input or output data. See *below* {learn more}.

Note: You can use **Note** to add a concise comment about this function, if this is not apparent from the software description and EDAM annotations.

Tip: When deciding how to describe your tools, in terms of *bio.tools* entries, their functions and operations, always keep the end-user in mind and try to describe your tools in a way that will be clear to them.

It can be difficult to find the right terms to describe a tools operation(s), input(s) or output(s). It's highly recommended to use EDAM Tool Annotator to describe the function, and carefully copy-paste the JSON ouput (in the bottom pane of the window) into the *JSON* tab of the *bio.tools editing interface*. Or use the OLS, BioPortal or EDAM Browser alongside *bio.tools* when describing your tools. If you're not sure, mail registry-support for help.

Operation

Before describing your tools, you should carefully identify the distinct functions and the individual operations associated with each one. This is often straighforward, as different functions (modes) typically perform distinct operations:

• if a tool has an option between doing one thing or another, then you should annotate the operations as distinct functions

- if in contrast a tool always does one or more things, then you should annotate these as distinct operations within a single function
- only specify the primary functions and operations, from a typical end-user perspective tools often do many other things than its central, advertised purpose you don't need to describe everything!

Data

- data terms must be correctly associated with the operation(s)
- only specify the primary inputs and outputs, *e.g.* a sequence alignment tool would be annotated as reading sequences (input), and writing a sequence alignment (output), but not with gap insertion and extension penalties, or other parameters.

Format

- format terms must be correctly associated with an input or output data type
- specify the most widely used of the supported data formats it can be impractical / onerous to be exhaustive!

Other fields

Other sections in the *bio.tools* editing interface include:

- *Labels* specify miscellaneous scientific, technical and administrative details, expressed in terms from controlled vocabularies. {learn more}
- *Links* specify miscellaneous links for the tool. The type of information obtained when resolving the link is specified by *Link type*. {learn more}
- Download specify links to downloads for your software. {learn more}
- *Documentation* link to documentation about the software. {learn more}
- *Publications* specify publications about the software. {learn more}
- *Credits & Support* specify individuals or organisations that should be credited, or may be contacted about the software. Credits include all type of entities that contributed to the development, maintenance or provision of the resource. {learn more}
- *Relations* specify details of a relationship this software shares with other software registered in *bio.tools*. {learn more}

CHAPTER 7

Editors Guide

Thematic editors are registry-dev members responsible for overseeing coverage and quality in specific thematic areas. The editorships will enable expanding accurate high-standard software annotations in *bio.tools* to most scientific topics in the life sciences.

..note:: The concept of "thematic editors" is a work in progress which we will develop as funding and capacity permits.

7.1 Background

The sheer number of software and continuous advancements in tool development demand extensive and sustained efforts to provide comprehensive annotations. Such challenges can be overcome by distributing the curation effort across a network of engaged and experienced partners, which contribute to improve *bio.tools* content and to adjust the EDAM vocabulary (used in *bio.tools*) to the needs of the respective communities. Careful coordination of the distributed tasks is required to maintain quality standards and increase tool interoperability across the board.

Thematic editors are well connected with their respective scientific community, experts in their field, have a broad knowledge about commonly used software and are motivated to promote *bio.tools*. Editors normally oversee the work of one or more student curators, on a range of tasks to improve EDAM and *bio.tools* content:

- Review of *bio.tools* and EDAM to survey coverage of concepts, terms and tools.
- Help develop strategy to achieve and sustain a minimum information level in *bio.tools*, as per the emerging information standard.
- Engage with their community, supervise hackathons and promote *bio.tools* in general.
- · Mentor a student for practical curation work
- Implement sustainable procedures for systematic tool reviews and curation standards.

Benefits: A thematic editorships provides the opportunity to become a curation expert and contribute to a project for the benefit of the whole bioinformatics community. Editors will acquire extensive knowledge and experience about available software in their fields *e.g.* with opportunity to publish high-quality reviews. The editors will train additional experts during training and curation events (*e.g.* hackathons) as well as *via* student supervision. Moreover, the ELIXIR infrastructure will support them to amplify their activities within a broader context.

7.2 Candidate thematic editors

Editor	Topics
Anne Wenzel	RNA structure
Jon Ison	General purpose sequence analysis
Jose M. Carazo	Electron microscopy, structural biology
Josep Gelpi	Structural bioinformatics
Jurgen Haas	Protein structural biology, structural bioinformatics
Marta Villegas	Natural language processing
Martin Krallinger	Text Mining, natural language processing, named entity recognition
Reza Salek	Metabolomics
Veit Schwämmle	Proteomics, statistics
Vivi R. Gregersen	Agricultural science (association analysis, genomics)

We have expressions of interest from the following people:

People listed below, in the past served as EDAM Editors; we are aiming for a single, consolidated group of Thematic Edditors serving both EDAM and *bio.tools*.

Editor	Topics
David Sehnal	General bioinformatics
Dmitry Repchevsky	ES tools & services
Ivan Mičetić	Protein structure
Laura Emery	EBI tools and training
Lukáš Pravda	Structural bioinformatics
Stanislav Geidl	Chemoinformatics

bio.tools studentships can support thematic editors. A typical studentship comprises (at least) one full month of full working hours which are mostly distributed over a longer time period. Applications are written on basis of the template (see *e.g.* proteomics studentship). The students are recruited after proposal dissemination *via* GitHub, project mailing lists *etc*.

CHAPTER 8

API Reference

Attention:

- reference docs for the bio.tools API
- to make suggestions about these guidelines please add comments via GitHub
- if you find a bug, have any questions or suggestions, please get in touch with us.
- see also the API Usage Guide

The bio.tools Web API provides an easy way to access the bio.tools database.

8.1 List tools

List and search through all the available tools. Can sort, filter, and search the results.

HTTP GET

```
https://bio.tools/api/tool/
https://bio.tools/api/t/
```

8.1.1 Endpoint parameters

Pa- rame- ter	Re- quired	Туре	De- fault	Description
page	No	Integer	1	Result page number
format	No	String(json, api)	json	Response media type
q	No	String		Query term, used for searching, matches all at- tributes
sort	No	String(lastUpdate, additionDate, name, affiliation, score)	las- tUp- date	Sorts the results by choosen value (score only available when there is a query)
ord	No	String(desc, asc)	desc	Orders the results by either Ascending or De- scending order
<at- tribute></at- 	No	String		Filter by <attribute>. List of supported at- tributes below.</attribute>

8.1.2 Filtering

To filter the results by attribute name, the attribute name has to be added as a parameter to the URL, with the value being the desired search term, e.g. ?name=signalp

Attributes

These are the attributes supported by bio.tools:

Parameter	Search behaviour
biotoolsID	Search for bio.tools tool ID (usually quoted - to get ex-
	act match)
	biotoolsID="signalp"
name	Search for tool name (quoted as needed)
	name=signalp
homepage	Exact search for tool homepage URL (must be quoted)
	homepage="http://cbs.dtu.dk/services/SignalP/"
description	Search over tool description (quoted as needed)
	description="peptide cleavage"
version	Exact search for tool version (must be quoted)
	version="4.1"
topic	Search for EDAM Topic (term) (quoted as needed)
	topic="Proteomics"
topicID	Exact search for EDAM Topic (URI): must be quoted
	topicID="topic_3510"
function	Fuzzy search over function (input, operation, output,
	note and command)
	function="Sequence analysis"
operation	Fuzzy search for EDAM Operation (term) (quoted as
	needed)
	operation="Sequence analysis"
	Continued on payt page

Continued on next page

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Table 1 – continued from previous pa	ge
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Parameter	Search behaviour
outputDataFormatID	Exact search over output for EDAM Format (ID) (must
· · · · · · · · · · · · · · · · · · ·	be quoted)
	outputDataFormatID="format_1982"
toolType	Exact search for tool type
toorijpe	toolType="Command-line tool"
collectionID	Exact search for tool collection (normally quoted)
	collectionID="Rare Disease"
maturity	Exact search for tool maturity
macuity	maturity=Mature
operatingSystem	Exact search for tool operating system
operatingojstem	operatingSystem=Linux
language	Exact search for programming language
	language=Java
cost	Exact search for cost
	cost="Free of charge"
license	Exact search for software or data usage license (quoted
neense	as needed)
	license="GPL-3.0"
accessibility	Exact search for tool accessibility
	accessibility="Open access"
credit	Fuzzy search over credit (name, email, URL, ORCID
	iD, type of entity, type of role and note)
	credit="Henrik Nielsen"
creditName	Exact search for name of credited entity
	creditName="Henrik Nielsen"
creditTypeRole	Exact search for role of credited entity
	creditTypeRole=Developer
creditTypeEntity	Exact search for type of credited entity
J. J	creditTypeEntity="Funding agency"
creditOrcidID	Exact search for ORCID iD of credited entity (must be
	quoted)
	creditOrcidID="0000-0001-5121-2036"
publication	Fuzzy search over publication (DOI, PMID, PMCID,
-	publication type and tool version) (quoted as needed)
	publication=10.12688/f1000research.12974.1
publicationID	Exact search for publication ID (DOI, PMID or PM-
-	CID) (must be quoted)
	publicationID="10.12688/f1000research.12974.1"
publicationType	Exact search for publication type
	publicationType=Primary
publicationVersion	Exact search for tool version associated with a publica-
	tion (must be quoted)
	publicationVersion="1.0"
link	Fuzzy search over general link (URL, type and note)
	(quote as needed)
	link="Issue tracker"
	Exact search for type of information found at a link
linkType	Exact search for type of information found at a link

Table 1 – continued from previous page

Continued on next page

Parameter	Search behaviour
documentation	Fuzzy search over documentation link (URL, type and
	note) (quote as needed)
	documentation=Manual
documentationType	Exact search for type of documentation
	documentationType=Manual
download	Fuzzy search over download link (URL, type, version
	and note) (quote as needed)
	download=Binaries
downloadType	Exact search for type of download
	downloadType=Binaries
downloadVersion	Exact search for tool version associated with a down-
	load (must be quoted)
	downloadVersion="1.0"
otherID	Fuzzy search over alternate tool IDs (ID value, type of
	ID and version)
	otherID="rrid:SCR_015644"
otherIDValue	Exact search for value of alternate tool ID (must be
	quoted)
	otherIDValue="rrid:SCR_015644"
otherIDType	Exact search for type of alternate tool ID
	otherIDType=RRID
otherIDVersion	Exact search for tool version associated with an alter-
	nate ID (must be quoted)
	otherIDVersion="1.0"

Table 1 – continued from previous page

Important:

Values of the following parameters must be given in quotes to get sensible (or any) results:

- homepage
- version
- topicID
- operationID
- dataTypeID
- dataFormatID
- inputID
- inputDataTypeID
- inputDataFormatID
- outputID
- outputDataTypeID
- outputDataFormatID
- creditOrcidID
- publicationID
- publicationVersion

- downloadVersion
- otherIDValue
- otherIDVersion

e.g.

https://bio.tools/api/tool?topicID="topic_3510"

Values of other parameters can be quoted or unquoted:

- Unquoted values invoke a fuzzy word search: it will search for fuzzy matches of words in the search phrase, to the target field
- Quoted values invoke an exact phrase search; it will search for an exact match of the full-length of the search phrase, to the target field (matches to target substrings are allowed)

e.g.

- https://bio.tools/api/tool?biotoolsID="blast" returns the tool with biotoolsID of "blast" (the "canonical" blast)
- https://bio.tools/api/tool?biotoolsID=blast returns all tools with "blast" in their biotoolsID (all blast flavours)

Caution: The parameters are (currently) case-sensitive, *e.g.* you **must** use &biotoolsID= and not &biotoolsid

8.1.3 Example

Note:

An EDAM concept ID can be specified as a concept URI or ID:

- Concept URI e.g. http://edamontology.org/operation_2403
- Concept ID e.g. operation_2403

In future we may add support for:

- Concept CURIE e.g. EDAM: operation_2403
- Numerical ID e.g. 2403

Note: URIs and IDs must be quoted, e.g. &topicID="operation_2403"

8.1.4 Response data

Key Name	Description	Example
count	The total tool count results for your query	2313
previous	Link to the previous page	?page=4
next	Link to the next page ?	
list	An array with multiple tools and their relative information	ARRAY

8.2 Tool detail

Obtain information about a single tool.

HTTP GET

```
https://bio.tools/api/tool/:id/
https://bio.tools/api/t/:id/
https://bio.tools/api/:id/
```

8.2.1 Endpoint Parameters

Parameter	Required	Туре	Default	Description
id	Yes	String		biotoolsID
format	No	String(json, xml, api)	json	Response media type

8.2.2 Example

```
curl -X GET "https://bio.tools/api/tool/signalp/?format=json"
```

Caution: bio.tools supports upload/download of data in XML format compliant to biotoolsScheme v3.0.0. If you want to download in XML format you should use these endpoints (see Tool detail below):

```
https://bio.tools/api/tool/id/
https://bio.tools/api/t/id/
https://bio.tools/api/id/
```

e.g. https://bio.tools/api/tool/signalp

Were you to try to get XML format returned from a search over bio.tools

e.g. https://bio.tools/api/tool?toolid=signalp&format=xml

currently you'd get garbled / invalid XML (don't use it!) - we're looking at a fix.

8.3 Register a tool

Register a new tool.

Important: This method requires the user to be authenticated. Learn how to Log in / obtain token.

HTTP POST

```
https://bio.tools/api/tool/
https://bio.tools/api/t/
```

8.3.1 Endpoint Parameters

Parameter	Required	Туре	Description
data	Yes	Tool	Tool you wish to register. See an example tool.

Note: It is possible to specify editing permissions for tools. Learn how to manage *Editing permissions*.

8.3.2 Headers

Parameter	Re-	Allowed values	Description
	quired		
Content-	Yes	String(application/json, applica-	Media type
Туре		tion/xml)	
Authoriza-	Yes	String('Token <authorization td="" to-<=""><td>Authorization header. Learn how to Log in / ob-</td></authorization>	Authorization header. Learn how to Log in / ob-
tion		ken>')	tain token.

8.3.3 Example

```
curl -X POST -H "Content-Type: application/json" \
   -H "Authorization: Token 028595d682541e7e1a5dcf2306eccb720dadafd7" \
   -d '<resource>' "https://bio.tools/api/tool/"
```

8.4 Validate registering a tool

Test registering a tool without it actually being saved into the database.

Important: This method requires the user to be authenticated. Learn how to Log in / obtain token.

HTTP POST

```
https://bio.tools/api/tool/validate/
https://bio.tools/api/t/validate/
```

8.4.1 Endpoint Parameters

Parameter	Required	Туре	Description
data	Yes	Tool	Tool you wish to validate. See an example tool.

8.4.2 Headers

Parameter	Re-	Allowed values	Description
	quired		
Content-	Yes	String(application/json, applica-	Media type
Туре		tion/xml)	
Authoriza-	Yes	String('Token <authorization td="" to-<=""><td>Authorization header. Learn how to Log in / ob-</td></authorization>	Authorization header. Learn how to Log in / ob-
tion		ken>')	tain token.

8.4.3 Example

```
curl -X POST -H "Content-Type: application/json" \
  -H "Authorization: Token 028595d682541e7e1a5dcf2306eccb720dadafd7" \
  -d '<resource>' "https://bio.tools/api/tool/validate/"
```

8.5 Update a tool

Update a tool description.

Important: This method requires the user to be authenticated. Learn how to Log in / obtain token.

HTTP PUT

```
https://bio.tools/api/tool/:id/
https://bio.tools/api/t/:id/
https://bio.tools/api/:id/
```

8.5.1 Endpoint Parameters

Parameter	Required	Туре	Description
id	Yes	String	biotoolsID
data	Yes	Tool	Description with which you wish to update the tool See an example tool.

Note: It is possible to specify editing permissions for tools. Learn how to manage *Editing permissions*.

8.5.2 Headers

Parameter	Re- quired	Allowed values	Description
Content- Type	Yes	String(application/json, applica- tion/xml)	Media type
Authoriza- tion	Yes	String('Token <authorization to-<br="">ken>')</authorization>	Authorization header. Learn how to <i>Log in / ob-</i> <i>tain token</i> .

8.5.3 Example

```
curl -X PUT -H "Content-Type: application/json" \
   -H "Authorization: Token 028595d682541e7e1a5dcf2306eccb720dadafd7" \
   -d '<resource>' "https://bio.tools/api/tool/SignalP"
```

8.6 Validate updating a tool

Test updating a tool without it actually being saved into the database.

Important: This method requires the user to be authenticated. Learn how to Log in / obtain token.

HTTP PUT

```
https://bio.tools/api/tool/:id/validate/
https://bio.tools/api/t/:id/validate/
https://bio.tools/api/:id/validate/
```

8.6.1 Endpoint Parameters

Parame-	Re-	Туре	Description
ter	quired		
id	Yes	String	biotoolsID
data	Yes		Tool Description with which you wish to update the tool for validation See an example tool.

8.6.2 Headers

Parameter	Re-	Allowed values	Description
	quired		
Content-	Yes	String(application/json, applica-	Media type
Туре		tion/xml)	
Authoriza-	Yes	String('Token <authorization td="" to-<=""><td>Authorization header. Learn how to Log in / ob-</td></authorization>	Authorization header. Learn how to Log in / ob-
tion		ken>')	tain token.

8.6.3 Example

```
curl -X PUT -H "Content-Type: application/json" \
   -H "Authorization: Token 028595d682541e7e1a5dcf2306eccb720dadafd7" \
   -d '<resource>' "https://bio.tools/api/tool/SignalP/validate/"
```

8.7 Editing permissions

Manage editing permissions for the registered tools.

There are currently three types of editing permissions supported by the system:

8.7.1 Private

A private tool can only be edited by the creator of the tool. This is the default option. In order to set this kind of permission, add the following info into the tool data:

```
"editPermission": {
    "type": "private"
}
```

8.7.2 Public

Public tool can be modified by any user registered in the system. In order to set this kind of permission, add the following info into the tool data:

```
"editPermission": {
    "type": "public"
}
```

8.7.3 Group

Specify a list of users in the system that can edit the tool. In order to set this kind of permission, add the following info into the tool data:

```
"editPermission": {
    "type": "private",
    "authors": [
        "registered_user_1", "registered_user_2"
    ]
}
```

8.8 Delete a tool

Removes a tool from the registry.

Important: This method requires the user to be authenticated. Learn how to Log in / obtain token.

HTTP DELETE

```
https://bio.tools/api/tool/:id/
https://bio.tools/api/t/:id/
https://bio.tools/api/:id/
```

8.8.1 Endpoint Parameters

Parameter	Required	Туре	Description
id	Yes	String	biotoolsID

8.8.2 Headers

Parameter	Re-	Allowed values	Description
	quired		
Authoriza-	Yes	String('Token <authorization td="" to-<=""><td>Authorization header. Learn how to Log in / obtain</td></authorization>	Authorization header. Learn how to Log in / obtain
tion		ken>')	token.

8.8.3 Example

```
curl -X DELETE \
-H "Authorization: Token 028595d682541e7e1a5dcf2306eccb720dadafd7" \
"https://bio.tools/api/tool/SignalP"
```

8.9 List used terms

Obtain a list of terms registered with tools for some attributes, e.g. a list of names of all tools.

HTTP GET

```
https://bio.tools/api/used-terms/:attribute
```

8.9.1 Endpoint Parameters

Param-	Re-	Туре	De-	Description
eter	quired		fault	
at-	Yes	String(name, topic, functionName, input,		Attribute for which a list of used terms
tribute		output, credits, all)		will be returned
format	No	String(json, xml, api)	json	Response media type

8.9.2 Example

curl -X GET "https://bio.tools/api/used-terms/name/?format=json"

8.9.3 Response data

Key Name	Description
data	A list of used terms

8.10 Create a user account

Creates a user account and emails a verification email.

HTTP POST

```
https://bio.tools/api/rest-auth/registration/
```

8.10.1 POST data

Key	Re-	Туре	Description	Example
Name	quired			
username	Yes	String	Account username	username
pass-	Yes	String	Password	password
word1				
pass-	Yes	String	Repeated password	password
word2				
email	Yes	String	Account email. The verification email will be sent to this	exam-
			address	ple@example.org

8.10.2 Headers

Parameter	Required	Allowed values	Description
Content-Type	Yes	String(application/json, application/xml)	POST data media type

8.10.3 Example

```
curl -X POST -H "Content-Type: application/json" \
  -d '{"username":"username", "password1":"password", \
  "password2":"password", "email":"example@example.org"}' \
  "https://bio.tools/api/rest-auth/registration/"
```

8.11 Verify a user account

Verifies a user account based on the emailed verification key.

HTTP POST

https://bio.tools/api/rest-auth/registration/verify-email/

8.11.1 POST data

Key	Re-	Туре	Description	Example	
Name	quired				
key	Yes	String	Verification key from account	ndwowtbpmlk5zxdxfrwgu2822xynjidhizhwosycve7h	olof156hjwdsf1f
			creation email		

8.11.2 Headers

Parameter	Required	Allowed values	Description
Content-Type	Yes	String(application/json, application/xml)	POST data media type

8.11.3 Example

```
curl -X POST -H "Content-Type: application/json" \
  -d '{"key":"ndwowtbpmlk5zxdxfrwgu2822xynjidhizhwosycve7hro1of156hjwdsf1f6gbn"}' \
  "https://bio.tools/api/rest-auth/registration/verify-email/"
```

8.12 Log in / obtain token

Logs the user in and returns an authentication token.

HTTP POST

```
https://bio.tools/api/rest-auth/login/
```

8.12.1 POST data

Key Name	Required	Туре	Description	Example
username	Yes	String	Account username	username
password	Yes	String	Password	password

8.12.2 Headers

Parameter	Required	Allowed values	Description
Content-Type	Yes	String(application/json, application/xml)	POST data media type

8.12.3 Example

```
curl -X POST -H "Content-Type: application/json" \
 -d '{"username":"username","password":"password"}' \
"https://bio.tools/api/rest-auth/login/"
```

8.12.4 Response data

Key Name	Description
key	Authentication token

8.13 Get user information

Return information about the logged in user account, including a list of registered tool (name, id, version, addition-Date, lastUpdate)

Important: This method requires the user to be authenticated. Learn how to Log in / obtain token.

HTTP GET

```
https://bio.tools/api/rest-auth/user/
```

8.13.1 Endpoint Parameters

Parameter	Required	Туре	Default	Description
format	No	String(json, xml, api)	json	Response media type

8.13.2 Headers

Parameter	Re-	Allowed values	Description
	quired		
Authoriza-	Yes	String('Token <authorization td="" to-<=""><td>Authorization header. Learn how to Log in / obtain</td></authorization>	Authorization header. Learn how to Log in / obtain
tion		ken>')	token.

8.13.3 Example

```
curl -X GET \
  -H "Authorization: Token 028595d682541e7e1a5dcf2306eccb720dadafd7" \
  "https://bio.tools/api/rest-auth/user/?format=json"
```

8.13.4 Response data

Key Name	Description		
username	Account username		
email	Account email		
resources	List of registered tools (limited to name, id, version, additionDate, lastUpdate)		

8.14 Log out

Log out of the system.

Important: This method requires the user to be authenticated. Learn how to Log in / obtain token.

HTTP POST

https://bio.tools/api/rest-auth/logout/

8.14.1 Headers

Parameter	Re-	Allowed values	Description
	quired		
Authoriza-	Yes	String('Token <authorization td="" to-<=""><td>Authorization header. Learn how to Log in / obtain</td></authorization>	Authorization header. Learn how to Log in / obtain
tion		ken>')	token.

8.14.2 Example

```
curl -X POST
-H "Authorization: Token 028595d682541e7e1a5dcf2306eccb720dadafd7" \
"https://bio.tools/api/rest-auth/logout/"
```

8.15 Reset user password

Send a password reset email.

HTTP POST

```
https://bio.tools/api/rest-auth/password/reset/
```

8.15.1 POST data

Key Name	Required	Туре	Description	Example
email	Yes	String	Account email	example@example.org

8.15.2 Headers

Parameter	Required	Allowed values	Description
Content-Type	Yes	String(application/json, application/xml)	POST data media type

8.15.3 Example

```
curl -X POST -H "Content-Type: application/json" \
  -d '{"email":"example@example.org"}' \
  "https://bio.tools/api/rest-auth/password/reset/"
```

8.16 Confirm password reset

Confirm a password reset using uid and token from a password reset email.

HTTP POST

```
https://bio.tools/api/rest-auth/password/reset/confirm/
```

8.16.1 POST data

Key Name	Required	Туре	Description	Example
uid	Yes	String	UID from password reset email	MQ
token	Yes	String	Token from password reset email	4ct-67e90a1ab4f22fbb9b9f
password1	Yes	String	New password	new_password
password2	Yes	String	New password repeated	new_password

8.16.2 Headers

Parameter	Required	Allowed values	Description
Content-Type	Yes	String(application/json, application/xml)	POST data media type

8.16.3 Example

```
curl -X POST -H "Content-Type: application/json" \
-d '{"uid":"MQ", "token":"4ct-67e90alab4f22fbb9b9f", \
"password1":"new_password", "password2":"new_password"}' \
"https://bio.tools/api/rest-auth/password/reset/confirm/"
```

8.17 Stats

Compile stats about a the registry.

HTTP GET

```
https://bio.tools/api/stats
```

8.17.1 Example

curl -X GET "https://bio.tools/api/stats"

CHAPTER 9

API Usage Guide

Attention:

- guidelines for the bio.tools API
- to make suggestions about these guidelines please add comments via GitHub
- see also the API Reference

bio.tools implements the model of software information defined in biotoolsScheme v3.0.0 . This page summarises the structure and syntax of an XML / JSON file that describes a tool for submission to bio.tools via the API.

9.1 Payload formats

To submit a tool via the bio.tools API you'll need to POST a tool description to the tool endpoint. The API supports XML and JSON format uploads and downloads comatible with biotoolsSchema.

Note: Support for YAML (and other) formats can be added if required. If you want this, please tell us via GitHub.

9.1.1 XML

See the sample XML document.

Important: When working in XML, please first read the biotoolsSchema docs. It is essential to stick to the element order (including nested elements) in the sample XML documents and as shown below.

9.1.2 **JSON**

A sample JSON document may look like this:

```
{
  "name": "SignalP",
  "description": "Prediction of the presence and location of signal peptide cleavage.
→sites in amino acid sequences from different organisms.",
  "homepage": "http://cbs.dtu.dk/services/SignalP/",
  "biotoolsID": "signalp",
  "biotoolsCURIE": "biotools:signalp",
  "version":
  [
     "6.4.0.0",
     "1.1 - 1.4, 2.0-alpha, 2.0-beta-01 - 2.0-beta-04, 2.0.0"
  1
  "otherID":
  [
     {
        "value": "RRID:SCR_015644",
        "type": "rrid",
         "version": "4.1"
     },
     {
         "value": "doi:10.1007/978-1-4939-7015-5_6",
         "type": "doi"
         "version": "4.1"
     }
  1
  "function":
   [
      {
         "operation":
         [
            {
               "uri": "http://edamontology.org/operation_0418",
               "term": "Protein signal peptide detection"
            },
            {
               "uri": "http://edamontology.org/operation_0422",
               "term": "Protein cleavage site prediction"
            }
         ],
         "input":
         [
           {
             "data":
             {
                "uri": "http://edamontology.org/data_2044",
                "term": "Sequence"
             },
             "format":
             [
               {
                  "uri": "http://edamontology.org/format_1929",
                  "term": "FASTA"
               },
```

```
{
                  "uri": "http://edamontology.org/format_3008",
                  "term": "MAF"
               }
             ]
           }
         ],
         "output":
         [
            {
               "data":
               {
                  "uri": "http://edamontology.org/data_1277",
                  "term": "Protein features"
               },
               "format":
               [
                  {
                     "uri": "http://edamontology.org/format_2305",
                     "term": "GFF"
                  },
                                        {
                     "uri": "http://edamontology.org/format_3164",
                     "term": "GTrack"
                  },
               ]
            },
            {
               "data":
               {
                  "uri": "http://edamontology.org/data_2955",
                  "term": "Sequence report"
               },
               "format":
               ſ
                  {
                     "uri": "http://edamontology.org/format_2331",
                     "term": "HTML"
                  }
               1
            }
         1
         "note": "Predicts the presence and location of signal peptide cleavage sites.
⇔in amino acid sequences from different organisms.",
        "cmd": "--someOption",
     }
  ],
  "toolType":
  [
    "Command-line tool",
    "Web application"
  ],
  "topic":
  ſ
    {
       "uri": "http://edamontology.org/topic_0080",
       "term": "Sequence analysis"
```

```
},
  {
    "uri": "http://edamontology.org/topic_0078",
    "term": "Proteins"
  }
],
"operatingSystem":
[
  "Linux",
  "Mac"
],
"language":
[
  "ActionScript",
 "C"
],
"license": "Proprietary",
"collectionID":
[
 "CBS",
  "mytools"
],
"maturity": "Mature",
"cost": "Free of charge (with restrictions)",
"accessibility":
[
   "Open access",
],
"link":
[
  {
    "url": "http://www.cbs.dtu.dk/cgi-bin/sw_request?signalp",
    "type": "Repository",
    "note": "A comment goes here"
  },
  {
    "url": "http://www.cbs.dtu.dk/helpdesk",
    "type": "Helpdesk",
    "type": "Issue tracker",
    "note": "A comment goes here"
  }
],
"download":
[
  {
    "url": "http://www.cbs.dtu.dk/cgi-bin/sw_request?signalp",
    "type": "Source code",
    "note": "A comment goes here"
    "version": "1.4"
},
  {
    "url": "http://www.cbs.dtu.dk/cgi-bin/sw_request?signalp",
    "type": "Binaries",
    "note": "A comment goes here"
    "version": "1.4"
  }
],
```

```
"documentation":
[
  {
    "url": "http://www.cbs.dtu.dk/services/SignalP",
    "type": "General",
    "type": "Code of conduct",
    "note": "A comment goes here"
  },
 {
    "url": "http://www.cbs.dtu.dk/services/SignalP",
    "type": "Citation instructions",
    "note": "A comment goes here"
 }
],
"relation":
Γ
  {
    "biotoolsID": "needle",
    "type": "isNewVersionOf",
  },
 {
    "biotoolsID": "emboss",
    "type": "includedIn"
 }
],
"publication":
[
  {
     "doi": "10.1038/nmeth.1701",
     "pmid": "21959131",
     "pmcid": "21959131",
     "type": "Primary",
     "note": "A comment goes here",
     "version": "1.4"
 },
  {
     "doi": "10.1038/nmeth.1701",
     "pmid": "21959131",
     "pmcid": "21959131",
     "type": "Other",
     "note": "A comment goes here",
     "version": "1.4"
 }
],
"credit":
[
   {
      "name": "TN Petersen",
      "email": "test@email.com",
      "url": "http://someurl.org",
      "orcidid": "test",
      "gridid": "test",
      "rorid": "test",
      "fundrefid": "test",
      "typeEntity": "Person",
      "typeRole": "Developer",
      "note": "A comment goes here"
```

```
},
{
    "elixirPlatform", "Tools",
    },
    {
        "elixirNode", "Denmark"
    }
],
}
```

9.2 Tool attributes

9.2.1 Name

Canonical software name assigned by the software developer or service provider, e.g. "needle"

Attribute name name

Required Yes

Cardinality 1 only

Type String

Restrictions Min length: 1

Max length: 100

Pattern: $[\p{Zs}A-Za-z0-9+\,\,\-_:;()] *$

Example

```
# XML
<name>needle</name>
# JSON
"name": "needle"
```

Note:

- name may only contain space, uppercase and lowercase letters, decimal digits, plus symbol, period, comma, dash, underscore, colon, semicolon and parentheses.
- line feeds, carriage returns, tabs, leading and trailing spaces, and multiple spaces are not allowed / will be removed.
- see the curation guidelines.

9.2.2 Description

Textual description of the software, e.g. "needle reads two input sequences and writes their optimal global sequence alignment to file. It uses the Needleman-Wunsch alignment algorithm to find the optimum alignment (including gaps) of two sequences along their entire length. The algorithm uses a dynamic programming method to ensure the alignment is optimum, by exploring all possible alignments and choosing the best."

Attribute name description

Required Yes

Cardinality 1 only

Type String

Restrictions Min length: 10

Max length: 1000

Example

XML
<pre><description>needle reads two input sequences and writes their optimal global_</description></pre>
ightarrowsequence alignment to file. It uses the Needleman-Wunsch alignment algorithm to
\rightarrow find the optimum alignment (including gaps) of two sequences along their entire
→length. The algorithm uses a dynamic programming method to ensure the alignment is
→optimum, by exploring all possible alignments and choosing the best.
JSON
"description": "needle reads two input sequences and writes their optimal global
ightarrowsequence alignment to file. It uses the Needleman-Wunsch alignment algorithm to
\rightarrow find the optimum alignment (including gaps) of two sequences along their entire
→length. The algorithm uses a dynamic programming method to ensure the alignment is
ightarrowoptimum, by exploring all possible alignments and choosing the best."

Note:

- minimum 10 and maximum 1000 characters.
- line feeds, carriage returns, tabs, leading and trailing spaces, and multiple spaces are not allowed / will be removed.
- see the curation guidelines.

9.2.3 Homepage

Homepage of the software, or some URL that best serves this purpose, e.g. "http://emboss.openbio.org/rel/rel6/apps/needle.html"

Attribute name homepage

Required Yes

Cardinality 1

Type URL

Restrictions Pattern: http(s?)://[^\s/\$.?#].[^\s]*

Example

```
# XML
<homepage>http://emboss.open-bio.org/rel/rel6/apps/needle.html</homepage>
# JSON
"homepage": "http://emboss.open-bio.org/rel/rel6/apps/needle.html"
```

Note:

- a single valid URL is specified.
- see the curation guidelines.

9.2.4 biotoolsID

Unique ID (case insensitive) of the tool that is assigned upon registration of the software in bio.tools, normally identical to tool name, e.g. "needle".

Attribute name biotoolsID

Required No

Cardinality 0 or 1

Type String

Restrictions Pattern: [_\-.0-9a-zA-Z] *

Example

```
# XML
<biotoolsID>needle</biotoolsID>
```

```
# JSON
"biotoolsID": "needle"
```

Attention:

• a biotoolsID is set (and can only be changed) by bio.tools admin. It can be retrieved by API, but if specified in the payload to a PUT or POST request will be disregarded.

Note:

• the biotoolssID is a URL-safe and Linked-Data-safe derivative of (often identical to) the tool name. Allowed characters are uppercase and lowercase English letters (case insensitive!), decimal digits, hyphen, period, and underscore. Spaces can be preserved as underscore ("_").

• see the curation guidelines.

9.2.5 biotoolsCURIE

bio.tools CURIE (compact URI) based on the unique bio.tools ID of the tool, e.g. "biotools:needle"

```
Attribute name biotoolsCURIE
Required No
Cardinality 0 or 1
Type String
Restrictions Pattern: biotools: [_\-.0-9a-zA-Z] *
```

Example

```
# XML
<biotoolsCURIE>needle</biotoolsCURIE>
# JSON
```

Attention:

• a biotoolsCURIE is set (and can only be changed) by bio.tools admin. It can be retrieved by API, but if specified in the payload to a PUT or POST request will be disregarded.

Note:

- the bio.tools CURIE is simply the bio.tools tool ID with the prefix "biotools:".
- see the curation guidelines.

"biotoolsCURIE": "needle"

9.2.6 Version

Version information (typically a version number) of the software applicable to this bio.tools entry, e.g. "6.4.0.0"

Attribute name version

Required No

Cardinality 0 to many

Type String array

Restrictions Min length: 1

Max length: 100

Pattern: [\p{Zs}A-Za-z0-9+\., \-_:; ()] *

Example

```
# XML
<version>6.4.0.0</version>
<version>1.1 - 1.4, 2.0-alpha, 2.0-beta-01 - 2.0-beta-04, 2.0.0</version>
# JSON
"version":
[
   "6.4.0.0",
   "1.1 - 1.4, 2.0-alpha, 2.0-beta-01 - 2.0-beta-04, 2.0.0"
]
```

Note:

• name may only contain space, uppercase and lowercase English letters, decimal digits, plus symbol, period, comma, dash, colon, semicolon and parentheses.

- line feeds, carriage returns, tabs, leading and trailing spaces, and multiple spaces are not allowed / will be removed.
- see the curation guidelines.

9.2.7 Other IDs

A unique identifier of the software, typically assigned by an ID-assignment authority other than bio.tools, e.g. "RRID:SCR_015644"

Attribute name otherID

Required No

Cardinality 0 to many

Type List of otherID objects

otherID object definition

- value
 - Required: Yes
 - Cardinality: 1 only
 - Type: String
 - Pattern: (doi|DOI):?10.[0-9]{4,9}[A-Za-z0-9:;\)\(_/.-]+
 - Pattern: (rrid|RRID):.+
 - Pattern: (cpe|CPE):.+
 - Pattern: (biotools|BIOTOOLS): [_\-.0-9a-zA-Z]*
- type
- Required: No
- Cardinality: 0 or 1
- Type: ENUM (list)
- Allowed values (see Curators Guide)
 - * doi
 - * rrid
 - * cpe
 - * biotoolsCURIE
- version
 - Required: No
 - Cardinality: 0 or 1
 - Type: String
 - Restrictions: Min length: 1, Max length: 100
 - Pattern: [\p{Zs}A-Za-z0-9+\., \-_:; ()] *

Example

```
# XML
<otherID>
      <value>RRID:SCR_015644</value>
      <type>rrid</type>
      <version>4.1</version>
</otherID>
<otherID>
      <value>doi:10.1007/978-1-4939-7015-5_6</value>
      <type>doi</type>
      <version>4.1</version>
</otherID>
# JSON
"otherID":
[
      {
          "value": "RRID:SCR_015644",
          "type:" "rrid",
          "version": "4.1"
      },
      {
          "value": "doi:10.1007/978-1-4939-7015-5_6",
          "type": "doi"
          "version": "4.1"
      }
]
```

Note:

- type can normally be inferred from the value but should be specified otherwise. In the example it was not actually necessary to specify "type".
- see the curation guidelines.

9.2.8 Function

Details of a function (i.e. mode of operation) the software provides, expressed in terms from the EDAM ontology.

Attribute name function

Required No

Cardinality 0 to many

Type List of function objects

Function object definition

Content

- Operation
 - Required: Yes
 - Cardinality: 1 to many
 - Type: List of EDAM objects
- Input

- Required: No
- Cardinality: 0 to many
- Type: List of input objects
- Output
 - Required: No
 - Cardinality: 0 to many
 - Type: List of output objects
- note
 - Required: No
 - Cardinality: 0 or 1
 - Type: String
 - Restrictions: min length: 10, max length: 1000
- cmd
 - Required: No
 - Cardinality: 0 or 1
 - Type: String
 - Restrictions: min length: 1, max length: 1000

Note:

- **note** and **cmd**: line feeds, carriage returns, tabs, leading and trailing spaces, and multiple spaces are not allowed / will be removed.
- see the curation guidelines for the function group, note and command.

Example

```
# XML
<function>
    <operation>
        <uri>http://edamontology.org/operation_0418</uri>
        <term>Protein signal peptide detection</term>
    </operation>
    <operation>
        <uri>http://edamontology.org/operation_0422</uri>
        <term>Protein cleavage site prediction</term>
    </operation>
    <input>
        <data>
          <uri>http://edamontology.org/data_2044</uri>
          <term>Sequence</term>
        </data>
        <format>
            <uri>http://edamontology.org/format_1929</uri>
            <term>FASTA</term>
        </format>
    <output>
```

```
<data>
          <uri>http://edamontology.org/data_1277</uri>
          <term>Protein features</term>
        </data>
        <format>
            <uri>http://edamontology.org/format_2305</uri>
            <term>GFF</term>
        </format>
        <data>
          <uri>http://edamontology.org/data_2955</uri>
          <term>Sequence report</term>
        </data>
        <format>
            <uri>http://edamontology.org/format_1929</uri>
            <term>FASTA</term>
        </format>
    </output>
    <note>Predicts the presence and location of signal peptide cleavage sites in_
⇔amino acid sequences from different organisms.</note>
    <cmd>-s best</cmd>
</function>
# JSON
"function":
[
  {
    "operation":
    [
      {
        "uri": "http://edamontology.org/operation_0418",
       "term": "Protein signal peptide detection"
      },
      {
        "uri": "http://edamontology.org/operation_0422",
        "term": "Protein cleavage site prediction"
     }
    ],
    "input":
    Γ
      {
        "data":
        {
          "uri": "http://edamontology.org/data_2044",
          "term": "Sequence"
        },
        "format":
        Γ
          {
            "uri": "http://edamontology.org/format_1929",
            "term": "FASTA"
          }
        ]
      }
    ],
    "output":
    Γ
```

```
{
        "data":
        {
          "uri": "http://edamontology.org/data_1277",
          "term": "Protein features"
        },
        "format":
        [
          {
            "uri": "http://edamontology.org/format_2305",
            "term": "GFF"
          }
        ]
     },
      {
        "data":
        {
          "uri": "http://edamontology.org/data_2955",
          "term": "Sequence report"
        },
        "format":
        [
          {
            "uri": "http://edamontology.org/format_1929",
            "term": "FASTA"
          }
       1
      }
   1
   "note": "Predicts the presence and location of signal peptide cleavage sites in_
→amino acid sequences from different organisms.",
   "cmd": "-s best",
  }
1
```

Operation

The basic operation(s) performed by this software function (EDAM Operation), e.g. "'Protein signal peptide detection' (http://edamontology.org/operation_0418)"

Attribute name operation

Required Yes

Cardinality 1 to many

Child of Function

Type List of EDAM objects

EDAM object definition

Content

• uri

- Required: No (if term present), Yes (otherwise)
- Cardinality: 0 or 1

- Type: URL
- term
 - Required: No (if URI present), Yes (otherwise)
 - Cardinality: 0 or 1
 - Type: String

Note:

- an EDAM ontology Operation concept URL and / or term are specified, *e.g.* "Multiple sequence alignment", http://edamontology.org/operation_0492.
- URI and term are validated against EDAM ontology; if term and URI do not match, an error will be returned.
- synonyms of terms (as defined in EDAM) are accepted
- see the curation guidelines.

Example

```
# XML
<operation>
        <uri>http://edamontology.org/operation_0418</uri>
        <term>Protein signal peptide detection</term>
</operation>
<operation>
        <uri>http://edamontology.org/operation_0422</uri>
        <term>Protein cleavage site prediction</term>
</operation>
# JSON
"operation":
[
    {
        "uri": "http://edamontology.org/operation_0418",
        "term": "Protein signal peptide detection"
    },
    {
        "uri": "http://edamontology.org/operation_0422",
        "term": "Protein cleavage site prediction"
    }
```

Input

Primary input data (if any)Attribute name inputRequired NoCardinality 0 to manyChild of FunctionType List of input objectsInput object definition

Content

```
• data
```

- Required: Yes
- Cardinality: 1 only
- Type: EDAM object
- format
 - Required: No
 - Cardinality: 0 to many
 - Type: List of EDAM objects

Example

```
# XML
    <data>
      <uri>http://edamontology.org/data_2044</uri>
      <term>Sequence</term>
    </data>
    <format>
        <uri>http://edamontology.org/format_1929</uri>
        <term>FASTA</term>
    </format>
# JSON
"input":
[
  {
    "data":
    {
      "uri": "http://edamontology.org/data_2044",
      "term": "Sequence"
    },
    "format":
    [
      {
        "uri": "http://edamontology.org/format_1929",
        "term": "FASTA"
      }
    ]
  }
]
```

Output

Primary output data (if any) Attribute name output Required No Cardinality 0 to many Child of *Function* Type List of output objects

Output object definition

Content

- data
 - Required: Yes
 - Cardinality: 1 only
 - Type: EDAM object
- format
 - Required: No
 - Cardinality: 0 to many
 - Type: List of EDAM objects

Example

```
# XML
"output":
    <data>
      <uri>http://edamontology.org/data_2044</uri>
      <term>Sequence</term>
    </data>
    <format>
        <uri>http://edamontology.org/format_1929</uri>
        <term>FASTA</term>
    </format>
# JSON
"output":
[
  {
    "data":
    {
      "uri": "http://edamontology.org/data_2044",
      "term": "Sequence"
    },
    "format":
    [
      {
        "uri": "http://edamontology.org/format_1929",
        "term": "FASTA"
      }
    ]
  }
1
```

Data

EDAM Data concept, e.g. "'Sequence' (http://edamontology.org/data_2044)" Attribute name

data

Required Yes

Cardinality 1 only

Child of Input or Output

Type EDAM object

EDAM object definition

Content

- uri
- Required: No (if term present), Yes (otherwise)
- Cardinality: 0 or 1
- Type: URL
- term
 - Required: No (if URI present), Yes (otherwise)
 - Cardinality: 0 or 1
 - Type: String

Note:

- an EDAM ontology Data concept URL and / or term are specified, *e.g.* "Protein sequences", http:// edamontology.org/data_2976.
- URI and term are validated against EDAM ontology; if term and URI do not match, an error will be returned.
- synonyms of terms (as defined in EDAM) are accepted, however, the synonym will be replaced with main term.
- see the curation guidelines.

Example

Format

EDAM Format concept, e.g. "'FASTA' (http://edamontology.org/format_1929)"

Attribute name format

Required No

Cardinality 0 to many

Child of Input or Output

Type List of EDAM objects

EDAM object definition

Content

- uri
- Required: No (if term present), Yes (otherwise)
- Cardinality: 0 or 1
- Type: URL
- term
 - Required: No (if URI present), Yes (otherwise)
 - Cardinality: 0 or 1
 - Type: String

Note:

- an EDAM ontology Format concept URL and / or term are specified, *e.g.* "FASTA", http://edamontology.org/ format_1929.
- URI and term are validated against EDAM ontology; if term and URI do not match, an error will be returned.
- synonyms of terms (as defined in EDAM) are accepted, however, the synonym will be replaced with main term.
- see the curation guidelines.

Example

9.2.9 Tool type

The type of application software: a discrete software entity can have more than one type, e.g. "Command-line tool, Web application"

Attribute name toolType

Required No

Cardinality 0 to many

Type ENUM (list)

Allowed values (see Curators Guide)

- Bioinformatics portal
- Command-line tool
- Database portal
- Desktop application
- Library
- Ontology
- Plug-in
- Script
- SPARQL endpoint
- Suite
- Web application
- Web API
- Web service
- Workbench
- Workflow

Example

```
# XML
<toolType>Command-line tool</toolType>
<toolType>Web application</toolType>
# JSON
"toolType":
[
   "Command-line tool",
   "Web application"
]
```

Note:

• see the curation guidelines.

9.2.10 Topic

General scientific domain the software serves or other general category (EDAM Topic), e.g. "'Protein sites, features and motifs' (http://edamontology.org/topic_3510)"

Attribute name topic

Required No

Cardinality 0 to many

Type List of EDAM objects

EDAM object definition

Content

- uri
 - Required: No (if term present), Yes (otherwise)
 - Cardinality: 0 or 1
 - Type: URL
- term
 - Required: No (if URI present), Yes (otherwise)
 - Cardinality: 0 or 1
 - Type: String

Example

```
# XML
<topic>
  <uri>http://edamontology.org/topic_0605</uri>
  <term>Informatics</term>
</topic>
<topic>
  <uri>http://edamontology.org/topic_3303</uri>
  <term>Medicine</term>
</topic>
# JSON
"topic":
[
  {
    "uri": "http://edamontology.org/topic_0605",
    "term": "Informatics"
  },
  {
    "uri": "http://edamontology.org/topic_3303",
    "term": "Medicine"
  }
1
```

Note:

- an EDAM ontology Topic concept URL and / or term are specified, e.g. "Proteomics", http://edamontology.org/ topic_0121.
- URI and term are validated against EDAM ontology; if term and URI do not match, an error will be returned.
- synonyms of terms (as defined in EDAM) are accepted, however, the synonym will be replaced with main term.
- see the curation guidelines.

9.2.11 Operating system

The operating system supported by a downloadable software package, e.g. "Linux"

Attribute name operatingSystem

Required No

Cardinality 0 to many

Type ENUM (list)

Allowed values (see Curators Guide)

- Linux
- Windows
- Mac

Example

```
# XML
<operatingSystem>Linux</operatingSystem>
<operatingSystem>Mac</operatingSystem>
# JSON
"operatingSystem":
[
 "Linux",
 "Mac"
]
```

Note:

```
• see the curation guidelines.
```

9.2.12 Programming language

Name of programming language the software source code was written in, e.g. "C"

Attribute name language

Required No

Cardinality 0 to many

Type ENUM (list)

Allowed values (see Curators Guide) ActionScript, Ada, AppleScript, Assembly language, AWK, Bash, C, C#, C++, COBOL, ColdFusion, CWL, D, Delphi, Dylan, Eiffel, Forth, Fortran, Groovy, Haskell, Icarus, Java, JavaScript, Julia, JSP, LabVIEW, Lisp, Lua, Maple, Mathematica, MATLAB, MLXTRAN, NMTRAN, OCaml, Pascal, Perl, PHP, Prolog, PyMOL, Python, R, Racket, REXX, Ruby, SAS, Scala, Scheme, Shell, Smalltalk, SQL, Turing, Verilog, VHDL, Visual Basic, XAML, Other

Example

```
# XML
<language>Python</language>
<language>C</language>
```

JSON

"language": ["Python", "C"

Note:

• see the curation guidelines.

9.2.13 License

Software or data usage license, e.g. "GPL-3.0"

Attribute name license

Required No

Cardinality 0 or 1

Type ENUM

Allowed values (see Curators Guide) OBSD, AAL, ADSL, AFL-1.1, AFL-1.2, AFL-2.0, AFL-2.1, AFL-3. 0, AGPL-1.0, AGPL-3.0, AMDPLPA, AML, AMPAS, ANTLR-PD, APAFML, APL-1.0, APSL-1.0, APSL-1.1, APSL-1.2, APSL-2.0, Abstyles, Adobe-2006, Adobe-Glyph, Afmparse, Aladdin, Apache-1.0, Apache-1.1, Apache-2.0, Artistic-1.0, Artistic-1.0-Perl, Artistic-1. 0-cl8, Artistic-2.0, BSD-2-Clause, BSD-2-Clause-FreeBSD, BSD-2-Clause-NetBSD, BSD-3-Clause, BSD-3-Clause-Attribution, BSD-3-Clause-Clear, BSD-3-Clause-LBNL, BSD-3-Clause-No-Nuclear-License, BSD-3-Clause-No-Nuclear-License-2014, BSD-3-Clause-No-Nuclear-Warranty, BSD-4-Clause, BSD-4-Clause-UC, BSD-Protection, BSD-Source-Code, BSL-1.0, Bahyph, Barr, Beerware, BitTorrent-1. 0, BitTorrent-1.1, Borceux, CATOSL-1.1, CC-BY-1.0, CC-BY-2.0, CC-BY-2.5, CC-BY-3.0, CC-BY-4.0, CC-BY-NC-1.0, CC-BY-NC-2.0, CC-BY-NC-2.5, CC-BY-NC-3.0, CC-BY-NC-4.0, CC-BY-NC-ND-1.0, CC-BY-NC-ND-2.0, CC-BY-NC-ND-2.5, CC-BY-NC-ND-3. 0 CC-BY-NC-ND-4.0, CC-BY-NC-SA-1.0, CC-BY-NC-SA-2.0, CC-BY-NC-SA-2.5. CC-BY-NC-SA-3.0, CC-BY-NC-SA-4.0, CC-BY-ND-1.0, CC-BY-ND-2.0, CC-BY-ND-2. 5, CC-BY-ND-3.0, CC-BY-ND-4.0, CC-BY-SA-1.0, CC-BY-SA-2.0, CC-BY-SA-2.5, CC-BY-SA-3.0, CC-BY-SA-4.0, CC0-1.0, CDDL-1.0, CDDL-1.1, CECILL-1.0, CECILL-1. 1, CECILL-2.0, CECILL-2.1, CECILL-B, CECILL-C, CNRI-Jython, CNRI-Python, CNRI-Python-GPL-Compatible, CPAL-1.0, CPL-1.0, CPOL-1.02, CUA-OPL-1.0, Caldera, ClArtistic, Condor-1.1, Crossword, CrystalStacker, Cube, D-FSL-1.0, DOC, DSDP, Dotseqn, ECL-1.0, ECL-2.0, EFL-1.0, EFL-2.0, EPL-1.0, EUDatagrid, EUPL-1.0, EUPL-1. 1, Entessa, ErlPL-1.1, Eurosym, FSFAP, FSFUL, FSFULLR, FTL, Fair, Frameworx-1.0, FreeImage, GFDL-1.1, GFDL-1.2, GFDL-1.3, GL2PS, GPL-1.0, GPL-2.0, GPL-3.0, Giftware, Glide, Glulxe, HPND, HaskellReport, IBM-pibs, ICU, IJG, IPA, IPL-1.0, ISC, ImageMagick, Imlib2, Info-ZIP, Intel, Intel-ACPI, Interbase-1.0, JSON, JasPer-2.0, LAL-1.2, LAL-1.3, LGPL-2.0, LGPL-2.1, LGPL-3.0, LGPLLR, LPL-1.0, LPL-1.02, LPPL-1.0, LPPL-1. 1, LPPL-1.2, LPPL-1.3a, LPPL-1.3c, Latex2e, Leptonica, LiLiQ-P-1.1, LiLiQ-R-1.1, LiLiQ-Rplus-1.1, Libpng, MIT, MIT-CMU, MIT-advertising, MIT-enna, MIT-feh, MITNFA, MPL-1.0, MPL-1.1, MPL-2.0, MPL-2.0-no-copyleft-exception, MS-PL, MS-RL, MTLL, MakeIndex, MirOS, Motosoto, Multics, Mup, NASA-1.3, NBPL-1.0, NCSA, NGPL, NLOD-1.0, NLPL, NOSL, NPL-1.0, NPL-1.1, NPOSL-3.0, NRL, NTP, Naumen, NetCDF, Newsletr, Nokia, Noweb, Nunit, OCCT-PL, OCLC-2.0, ODbL-1.0, OFL-1.0, OFL-1.1, OGTSL, OLDAP-1.1, OLDAP-1.2, OLDAP-1.3, OLDAP-1.4, OLDAP-2.0, OLDAP-2.0.1, OLDAP-2.1, OLDAP-2.2, OLDAP-2.2.1, OLDAP-2.2.2, OLDAP-2.3, OLDAP-2.4, OLDAP-2.5, OLDAP-2.6, OLDAP-2.7, OLDAP-2.8, OML, OPL-1.0, OSET-PL-2.1, OSL-1.0, OSL-1.1, OSL-2.0, OSL-2.1, OSL-3.0, OpenSSL, PDDL-1.0, PHP-3.0, PHP-3.01, Plexus, PostgreSQL, Python-2.0, QPL-1.0, Qhull, RHeCos-1.1, RPL-1.1, RPL-1.5, RPSL-1.0, RSA-MD, RSCPL, Rdisc, Ruby, SAX-PD, SCEA, SGI-B-1.0, SGI-B-1.1, SGI-B-2.0, SISSL, SISSL-1.2, SMLNJ, SMPPL, SNIA, SPL-1.0, SWL, Saxpath, Sendmail, SimPL-2.0, Sleepycat, Spencer-86, Spencer-94, Spencer-99, SugarCRM-1.1.3, TCL, TMate, TORQUE-1.1, TOSL, UPL-1.0, Unicode-TOU, Unlicense, VOSTROM, VSL-1.0, Vim, W3C, W3C-19980720, WTFPL, Watcom-1.0, Wsuipa, X11, XFree86-1.1, XSkat, Xerox, Xnet, YPL-1.0, YPL-1.1, ZPL-1.1, ZPL-2.0, ZPL-2.1, Zed, Zend-2.0, Zimbra-1.3, Zimbra-1.4, Zlib, bzip2-1.0.5, bzip2-1.0.6, curl, diffmark, dvipdfm, eGenix, gSOAP-1.3b, gnuplot, iMatix, libtiff, mpich2, psfrag, psutils, xinetd, xpp, zlib-acknowledgement, Proprietary, Freeware, Other, Not licensed

Example

```
# XML
<license>Proprietary</license>
# JSON
"license": "Proprietary"
```

Note:

• see the curation guidelines.

9.2.14 Collection

Unique ID of a collection that the software has been assigned to within bio.tools, e.g. "CBS

Attribute name collectionID

Required No

Cardinality 0 to many

Type List of strings

Restrictions Min length: 1

Max length: 100

Pattern: $[\p{Zs}A-Za-z0-9+\, \, \] *$

Example

```
# XML
<collectionID>CBS</collectionID>
<collectionID>NorduGrid</collectionID>
# JSON
"collectionID":
[
"CBS",
"NorduGrid"
]
```

Note:

- collection may only contain space, uppercase and lowercase letters, decimal digits, plus symbol, period, comma, dash, underscore, colon, semicolon and parentheses.
- line feeds, carriage returns, tabs, leading and trailing spaces, and multiple spaces are not allowed / will be removed.
- see the curation guidelines.

9.2.15 Maturity

How mature the software product is, e.g. "Mature"

Attribute name maturity

Required No

Cardinality 0 or 1

Type ENUM

Allowed values (see Curators Guide)

- Emerging
- Mature
- Legacy

Example

```
# XML
<maturity>Mature</maturity>
# JSON
"maturity": "Mature"
```

Note:

• see the curation guidelines.

9.2.16 Cost

Monetary cost of acquiring the software, e.g. "Free of charge (with retritions)"

Attribute name cost

Required No

Cardinality 0 or 1

Type ENUM

Allowed values (see Curators Guide)

- Free of charge
- Free of charge (with restrictions)

• Commercial

Example

```
# XML
<cost>Free of charge (with restrictions)</cost>
# JSON
"cost": "Free of charge (with restrictions)"
```

Note:

• see the curation guidelines.

9.2.17 Accessibility

Whether there are non-monetary restrictions on accessing an online service, e.g. "Open access"

Attribute name accessibility

Required No

Cardinality 0 or 1

Type ENUM (list)

Allowed values (see Curators Guide)

- Open access
- Open access (with restrictions)
- Restricted access

Example

```
# XML
<accessibility>Open access</accessibility>
# JSON
"accessibility":
[
```

"Open access",

Note:

1

• see the curation guidelines.

9.2.18 ELIXIR platform

ELIXIR platform credited for developing or providing the software.

Attribute name elixirPlatform

Required No

Cardinality 0 to many

Type ENUM (list)

Allowed values (see Curators Guide)

- Data
- Tools
- Compute
- Interoperability
- Training

Example

```
# XML
<elixirPlatform>Open access</elixirPlatform>
<elixirPlatform>Freeware</elixirPlatform>
# JSON
"elixirPlatform":
[
    "Tools",
    "Compute"
]
```

Note:

```
• see the curation guidelines.
```

9.2.19 ELIXIR node

ELIXIR node credited for developing or providing the software - the software is in Node Service Delivery Plan.

Attribute name elixirNode

Required No

Cardinality 0 to many

Type ENUM (list)

Allowed values (see Curators Guide)

- Belgium
- Czech Republic
- Denmark
- EMBL
- Estonia
- Finland
- France
- Germany
- Greece

- Hungary
- Ireland
- Israel
- Italy
- Luxembourg
- Netherlands
- Norway
- Portugal
- Slovenia
- Spain
- Sweden
- Switzerland
- UK

Example

```
# XML
<elixirNode>Denmark</elixirNode>
<elixirNode>France</elixirNode>
# JSON
"elixirNode":
[
   "Denmark",
   "France"
]
```

Note:

• see the curation guidelines.

9.2.20 ELIXIR community

ELIXIR (or associated) community to which the software is relevant.

Attribute name elixirCommunity

Required No

Cardinality 0 to many

Type ENUM (list)

Allowed values (see Curators Guide)

- 3D-BioInfo
- Federated Human Data
- Galaxy
- Human Copy Number Variation

- Intrinsically Disordered Proteins
- Marine Metagenomics
- Metabolomics
- Microbial Biotechnology
- Plant Sciences
- Proteomics
- Rare Diseases

Example

```
# XML
<elixirCommunity>Galaxy</elixirCommunity>
<elixirCommunity>Metabolomics</elixirCommunity>
# JSON
"elixirCommunity":
[
    "Galaxy",
    "Metabolomics"
]
```

Note:

• see the curation guidelines.

9.2.21 Link

Miscellaneous links for the software e.g. repository, issue tracker or mailing list.

Attribute name link

Required No

Cardinality 0 to many

Type List of link objects

Link object definition

Content

• url

- Required: Yes
- Cardinality: 1 only
- Type: URL
- Pattern: http(s?)://[^\s/\$.?#].[^\s]*
- type
 - Required: Yes
 - Cardinality: 1 or more
 - Type: ENUM

- Allowed values: (see Curators Guide)
 - * Discussion forum
 - * Galaxy service
 - * Helpdesk
 - * Issue tracker
 - * Mailing list
 - * Mirror
 - * Software catalogue
 - * Repository
 - * Service
 - * Social media
 - * Technical monitoring
 - * Other

• note

- Required: No
- Cardinality: 0 or 1
- Type: String
- Restrictions: min length: 10, max length: 1000

Example

```
# XML
<link>
<url>http://www.cbs.dtu.dk/cgi-bin/sw_request?signalp</url>
<type>Helpdesk</type>
<type>Issue tracker</type>
<note>A comment goes here.</note>
</link>
# JSON
"link":
[
  {
    "url": "http://www.cbs.dtu.dk/cgi-bin/sw_request?signalp",
    "type": "Helpdesk",
    "type": "Issue tracker",
    "note": "A comment goes here."
  }
]
```

Note:

- the note is minimum 10 and maximum 1000 characters. Line feeds, carriage returns, tabs, leading and trailing spaces, and multiple spaces are not allowed / will be removed.
- see the curation guidelines.

9.2.22 Download

Links to downloads for the software, e.g. source code, virtual machine image or container.

Attribute name download

Required No

Cardinality 0 to many

Type List of download objects

Download object definition

Content

• url

- Required: Yes
- Cardinality: 1 only
- Type: URL
- Pattern: http(s?)://[^\s/\$.?#].[^\s]*
- type
 - Required: Yes
 - Cardinality: 1 only
 - Type: ENUM
 - Allowed values: (see Curators Guide)
 - * API specification
 - * Biological data
 - * Binaries
 - * Command-line specification
 - * Container file
 - * Icon
 - * Screenshot
 - * Source code
 - * Software package
 - * Test data
 - * Test script
 - * Tool wrapper (CWL)
 - * Tool wrapper (galaxy)
 - * Tool wrapper (taverna)
 - * Tool wrapper (other)
 - * VM image
 - * Downloads page
 - * Other

• note

- Required: No
- Cardinality: 0 or 1
- Type: String
- Restrictions: min length: 10, max length: 1000

version

- Required: No
- Cardinality: 0 or 1
- Type: String
- Restrictions: Min length: 1, Max length: 100
- Pattern: [\p{Zs}A-Za-z0-9+\., \-_:; ()] *

Example

```
# XML
<download>
<url>http://www.cbs.dtu.dk/cgi-bin/sw_request?signalp</url>
<type>Source code</url>
<note>Complete distibution</note>
<version>1.4</version>
</download>
# JSON
"download":
[
  {
    "url": "http://www.cbs.dtu.dk/cgi-bin/sw_request?signalp",
    "type": "Source code",
    "note": "Complete distibution",
    "version": "1.4"
  }
]
```

Note:

- the note is minimum 10 and maximum 1000 characters. Line feeds, carriage returns, tabs, leading and trailing spaces, and multiple spaces are not allowed / will be removed.
- see the curation guidelines.

9.2.23 Documentation

Links to documentation about the software e.g. user manual, API documentation or training material.

Attribute name documentation

Required No

Cardinality 0 to many

Type List of documentation objects

Documentation object definition

Content

• url

- Required: Yes
- Cardinality: 1 only
- Type: URL
- Pattern: http(s?)://[^\s/\$.?#].[^\s]*
- type
 - Required: Yes
 - Cardinality: 1 or more
 - Type: ENUM
 - Allowed values: (see Curators Guide)
 - * API documentation
 - * Citation instructions
 - * Code of conduct
 - * Command-line options
 - * Contributions policy
 - * FAQ
 - * General
 - * Governance
 - * Installation instructions
 - * User manual
 - * Terms of use
 - * Release notes
 - * Training material
 - * Other
- note
 - Required: No
 - Cardinality: 0 or 1
 - Type: String
 - Restrictions: min legth:10, max length: 1000

Example

Note:

- the note is minimum 10 and maximum 1000 characters. Line feeds, carriage returns, tabs, leading and trailing spaces, and multiple spaces are not allowed / will be removed.
- see the curation guidelines.

9.2.24 Relation

Details of a relationship this software shares with other software registered in bio.tools.

Attribute name relation

Required No

Cardinality 0 to many

Type List of relation objects

Relation object definition

Content

- biotoolsID
 - Required: Yes
 - Cardinality: 1 only
 - Type: String
 - **– Pattern:** [_\-.0-9a-zA-Z] *

• type

- Required: Yes
- Cardinality: 1 only
- Type: ENUM
- Allowed values: (see Curators Guide)
 - * isNewVersionOf
 - * hasNewVersion

- * uses
- * usedBy
- * includes
- * includedIn

Example

```
# XML
<relation>
<biotoolsID>needle</biotoolsID>
<type>isNewVersionOf</type>
</relation>
# JSON
"relation":
[
  {
    "biotoolsID": "needle",
    "type": "isNewVersionOf",
  },
  {
    "biotoolsID": "emboss",
    "type": "includedIn",
  },
]
```

Note:

• see the curation guidelines.

9.2.25 Publication

Publications about the software

Attribute name publication

Required Yes

Cardinality 0 to many

Type List of publication objects

Publication object definition

Content

• pmcid

- Required: One of doi, pmid or pmcid must be specified.
- Cardinality: 0 or 1
- Type: PMCID
- **– Pattern:** (PMC) [1–9] [0–9] {0, 8}

• pmid

- Required: One of doi, pmid or pmcid must be specified.

- Cardinality: 0 or 1
- Type: PMID
- **–** Pattern: [1–9] [0–9] {0, 8}

• doi

- Required: One of doi, pmid or pmcid must be specified.
- Cardinality: 0 or 1
- Type: DOI
- Pattern: 10. [0-9] {4,9} [A-Za-z0-9:; \) \ (_/.-]+
- type
 - Required: No
 - Cardinality: 0 to many
 - Type: ENUM
 - Allowed values: (see Curators Guide) Primary Method Usage Benchmarking study Review Other
- note
 - Required: No
 - Cardinality: 0 or 1
 - Type: String
 - Restrictions: min length: 10, max length: 1000
- version
 - Required: No
 - Cardinality: 0 or 1
 - Type: String
 - Restrictions: Min length: 1, Max length: 100
 - Pattern: [\p{Zs}A-Za-z0-9+\., \-_:; ()]*

Example

(continued from previous page)

```
"pmid": "21959131",
"doi": "10.1038/nmeth.1701",
"type": "Primary",
"type": "Method",
"note": "A comment goes here",
"version": "4.0"
}
```

Note:

1

• see the curation guidelines.

9.2.26 Credit

Individuals or organisations that should be credited, or may be contacted about the software.

Attribute name credit

Required No

Cardinality 0 to many

Type List of credit objects

Credit object definition

Content

- name
 - Required: Yes
 - Cardinality: 0 or 1
 - Type: String
 - Restrictions: min length: 1, max length: 100
- orcidid
 - Required: No
 - Cardinality: 0 or 1
 - Type: String
 - Restrictions: pattern: http://orcid.org/{[]0-9]{4}-[0-9
 - Restrictions: pattern: https://orcid.org/{[]0-9]{4}-[0-
- gridid
 - Required: No
 - Cardinality: 0 or 1
 - Type: String
 - Restrictions: pattern: grid.[0-9]{4,}.[a-f0-9]{1,2}

rorid

- Required: No
- Cardinality: 0 or 1
- Type: String
- fundrefid
 - Required: No
 - Cardinality: 0 or 1
 - Type: String
- email
 - Required: No
 - Cardinality: 0 or 1
 - Type: Email
 - Restrictions: pattern: [A-Za-z0-9_]+([-+.'][A-Za-z0-9_]+)*@[A-Za-z0-9_]+([-.][A-Za-z0-9_]+([-.][A-Za-z0-9_]+)*
- url
- Required: No
- Cardinality: 0 or 1
- Type: URL
- Restrictions: pattern: http(s?)://[^s/\$.?#].[^s]*

• typeEntity

- Required: No
- Cardinality: 0 or 1
- Type: ENUM
- Allowed values: (see Curators Guide)
 - * Person
 - * Project
 - * Division
 - * Institute
 - * Consortium
 - * Funding agency

• typeRole

- Required: No
- Cardinality: 0 to many
- Type: ENUM (list)
- Allowed values: (see Curators Guide)
 - * Developer
 - * Maintainer

- * Provider
- * Documentor
- * Contributor
- * Support
- * Primary contact

• note

- Required: No
- Cardinality: 0 or 1
- Type: String
- Restrictions: min length: 10, max length: 1000

Example

```
# XML
<credit>
<name>TN Petersen</name>
<orcidid>http://orcid.org/0000-0002-1825-0097</orcidid>
<gridid>grid.5170.3</orcidid>
<rorid>03yrm5c26</rorid>
<fundrefid>10.13039/100009273</fundrefid>
<email>test@cbs.dtu.dk</email>
<url>http://cbs.dtu.dk</url>
<typeEntity>Person</typeEntity>
<typeRole>Developer</typeRole>
<typeRole>Documentor</typeRole>
<note>Lead developer</note>
</credit>
# JSON
"credit":
[
 {
    "name": "TN Petersen",
    "orcidid":"http://orcid.org/0000-0002-1825-0097",
    "gridid":"grid.5170.3",
    "rorid":"03yrm5c26",
   "fundrefid":"10.13039/100009273",
   "url": "http://cbs.dtu.dk",
    "email": "test@cbs.dtu.dk",
    "typeEntity": "Person",
    "typeRole":
    [
      "Developer",
      "Documentor"
    1
    "note": "Lead developer"
  }
]
```

Example

XML <credit>

(continues on next page)

(continued from previous page)

```
<elixirPlatform>Tools</elixirPlatform>
</credit>
# JSON
"credit":
[
{
    {
        "elixirPlatform": "Norway"
    }
]
```

Note:

- one of <name>, <email> or <url> must be specified.
- the credit name may only contain space, uppercase and lowercase letters, decimal digits, plus symbol, period, comma, dash, underscore, colon, semicolon and parentheses.
- line feeds, carriage returns, tabs, leading and trailing spaces, and multiple spaces are not allowed / will be removed.
- see the curation guidelines.

9.3 Entry management attributes

9.3.1 Permissions

Attribute name editPermission

Required No

Cardinality todo

Type Permission object

Permission object definition

Content

- type
 - Required: Yes
 - Cardinality: todo
 - Type: ENUM
 - Allowed values: private public group
- authors
 - Required: No
 - Cardinality: todo
 - Type: List of usernames

Notes 'authors' only need to be provided when type is set to group.

Example

```
# XML
# JSON
"editPermission":
{
    "type": "group",
    "authors":
    [
        "ekry",
        "lukbe"
    ]
}
```

Hangouts

Regular informal meetings to discuss all matters around *bio.tools* including ELIXIR EXCELERATE WP1 ("Tools Interoperability and Service Registry") tasks, activities of ELIXIR Denmark technical staff and partners.

You are welcome to suggest or attend a call; please mail Jon Ison (jison@bioinformatics.dtu.dk), including your gmail and skype addresses. To understand how we organise tasks and projects, read the Contributors Guide.

Roadmap

All developments of *bio.tools* software and content are informed by:

- 1. Community requests including partners and end-users.
- 2. Delivering priorities of the ELIXIR EXCELERATE grant (granted in April 2015) including revisions in light of 2017 midterm review.
- 3. Priorities of the ELIXIR Danish node.
- 4. Personal priorities of the *bio.tools* team, having insight of the core requirements.
- 5. Events on the ground.

For a summary of active issues see GitHub. We aim for quarterly major new releases of the production deployment (https://bio.tools) with new changes more regularly pushed to the development deployment (https://dev.bio.tools).

Tasks are assigned to quarterly milestones in GitHub. See in particular Critical and High priority issues and issues which are in progress.

Please join the discussion in GitHub. The *bio.tools* core team is very small, so bug fixes, new features *etc*. take a while - you're patience is appreciated!

For higher-level project management tasks, see https://biotools.sifterapp.com/ (for a sifter account mail Jon Ison).

bio.tools Studentships

ELIXIR Denmark - the coordinating node of the *bio.tools* project - earmars funds (as available) to support studentships to work on curation-focussed mini-projects for *bio.tools*. Projects must have clear and quantifiable impact on *bio.tools* content, in terms of number of entries and / or content quality. Projects can include developments of some tooling, so long as this contributes directly to the project goals.

If you would like to propose a project, then please discuss your ideas first by mailing Jon Ison cc Peter Longreen. If following this discussion, we all agree there is basis for a project, then we'd require a 1-page project proposal, the text of which we can work on together and in collaboration with other members of the registry-core group. Funding will be prioritised (by the Danish Node management) by proposals having the biggest potential impact on *bio.tools* content and quality.

We anticipate most projects to be short duration (normally the equivalent of a month full time work) however there is flexibility, especially where we find talented students who can clearly demonstrate that there work has made an impact. In case of project continuation, progress would be reviewed, and funding for projects that did not perform would be terminated.

12.1 Requirements

- each proposal requires (at least) two named mentors:
 - someone to vouch for the student, provide local on-site supervision, and handle payment of the student
 - someone (normally from the the registry-dev group) who will assist with supervision and oversee the delivery of the work
- students must be enrolled with an accedited University, or have accepted a place at such
- any tooling developed during the studentship would have to made freely available under open license

12.2 Answers to FAQ

• you are welcome to apply at any time

- there is no limit to the number of proposals, although a student can only be employed on one project at one time
- you cannot participate both as a mentor and a student
- only an individual may work on a project; groups cannot submit proposals
- when writing a proposal, please refer to the existing proposals below and follow the general structure and style
- projects must have clear and quantifiable impact on *bio.tools* content, but you are free to propose anything to these ends: you will need to inspect https://bio.tools and https://dev.bio.tools (latest dev server) to assess current status
- for futher information, mail Jon Ison cc Peter Longreen.
- we particularly welcome proposals from thematic editors.

12.3 Proposals

Finalised proposals are uploaded to https://github.com/bio-tools/Studentships/.

Mining the Scientific Literature for and Annotating Proteomics Software using the EDAM ontology and biotoolsXSD

STATUS: Complete. See Proposal. Open for comments.

Harvesting service descriptions for bio.tools using OpenAPI standards

STATUS: Complete. See Proposal.

See update on progress and pre-publication.

Annotating software tools in a scientific context

STATUS: Complete (5 students). See Proposal.

Annotating software tools in domains of the Life Sciences

STATUS: Funded and ongoing (metabolomics). Open for comments.

GitHub projects

There are now many subprojects concerning *bio.tools* and *EDAM*, including documentation, information scheman, adapters for file format conversion, shims for content import and export, utilities for text mining, and more.

.... The projects are nearly all hosted under the bio.tools and EDAM GitHub organisations:

- https://github.com/bio-tools
- https://github.com/edamontology/

Events

We have organised many events and regularly attend events organised by others. If you want to attend an event or have an idea for an event, please mail registry@elixir-dk.org. As a rule we try to avoid events in July & August. All attendees should please read our code of conduct.

- **Curation Hackathons** ("curatathons") gather providers from across the board to curate their resources, critique the Registry interfaces, and provide a forum for knowledge exchange and collaboration.
- **Thematic Hackathons** engage experts in a specific scientific area to help improve the relevant branches of EDAM, consolidate the existing registry annotations, as well as register new resources within the theme.
- **Resource Hackathons** collaborate with experts from a specific collection of tools and services, typically some other registry, community project or Web portal, to bring the collection up to the ELIXIR annotation standard and expose it in the Registry.
- **Technical Hackathons** focus on ontology, software or other technical developments in support of curation of the Registry, its technical development, applications and integration with other systems.

14.1 Forthcoming events

ELIXIR BioHackathon-Europe 2020 (Nov 9-13, 2020, Virtual) Following the success of the ELIXIR BioHackathon 2018 and BioHackathon 2019, this virtual edition will include multiple tracks related to bio.tools and EDAM:

- Project 10: EDAM and Tool Information Profiles
- Project 11: bio.tools integration and sustainable development

14.2 Past events

Hackathon: ELIXIR BioHackathon-Europe 2019 (Nov 18-22 2019, Campus des berges de Seine, FR)

https://2019.biohackathon-europe.org/

Scientific Software Registry Collaboration Workshop (Nov 13-14, 2019, Washington, USA)

https://asclnet.github.io/SWRegistryWorkshop/

Conference: ISMB/BOSC/CodeFest 2019 (Jul 21-27 2019, Basel, CH)

https://www.iscb.org/ismbeccb2019

https://www.open-bio.org/events/bosc-2019/

https://www.open-bio.org/events/bosc-2019/bosc-2019-collaborationfest/

Conference: GCC 2019 (Jul 1-6, Freiburg, DE)

https://galaxyproject.org/events/gcc2019/

GCC2019 was held in Freiburg, Germany, 1-6 July of 2019.

Conference: ELIXIR All-hands (Jun 17-20 2019, Lisbon, PT)

https://elixir-europe.org/events/elixir-excelerate-all-hands-meeting-2019

The fifth ELIXIR All Hands meeting took place 17-20 June 2019 in Lisbon. The meeting brings together members of the ELIXIR community from across the ELIXIR Nodes, and collaborators from partner organisations, in order to review ELIXIR's achievements and activities so far and discuss plans for the future. The All Hands meeting is also the venue for the ELIXIR-EXCELERATE Annual General Assembly Meeting.

Workshop: Debian Med 2019 Sprint (Mar 9-11 2019, Vilnius, ES)

https://wiki.debian.org/Sprints/2019/DebianMed2019

This is an informal co-working and co-learning event, participants are welcome to attend on the days that work for their schedule. EDAM and the integration of bio.tools with Debian Med and CWL was worked on.

Meeting: ELIXIR Tools Platform Face to Face Meeting (Jan 28 - 30 2019, Ghent, BE)

A more sustainable content management architecture, based on GitHub, was outlined in more detail. You can track developments on GitHub.

Hackathon: ELIXIR BioHackathon-Europe 2018 (Nov 12-16 2018, Campus des berges de Seine, FR)

The *bio.tools* and EDAM developers ran drop-in sessions each day of this 5-day hackathon, ranging from *bio.tools* testing and feature prioritisation, curation methods and tooling, through to prototyping a more sustainable content management architecture based on GitHub.

https://2018.biohackathon-europe.org/

Meeting: ELIXIR Tools and ELIXIR Compute Platforms : coordination (Sep 19 2018, Schipol, UK)

bio.tools was presented in context of a coordinated effort to establish ELIXIR-wide standards, protocols and processes for the orchestration of containerised applications and workloads provided by ELIXIR Communities.

Conference: ECCB 2018 - 17TH European Conference on Computational Biology (Sep 8-12 2018, Athens, GR)

http://eccb18.org/

Work on exploring the application of *bio.tools* data to automated workflow composition in mass spectrometry-based proteomics was presented. The work was recently published in Bioinformatics (10.1093/bioinformatics/bty646).

Conference: ELIXIR-DK @ 4th Annual Danish Bioinformatics Conference (Aug 29-30 2018, Odense, DK)

http://elixir-node.cbs.dtu.dk/?page_id=2369

This will showcase the work of the Danish ELIXIR node in context of the Danish and European bioinformatics community.

Conference: GCC-BOSC 2018 (Jun 25-30 2018, Portland, USA)

https://gccbosc2018.sched.com/list/descriptions/

The 2018 Galaxy Community Conference (GCC2018) and Bioinformatics Open Source Conference 2018 (BOSC2018) are meeting together in Portland, Oregon, United States, June 25-30, 2018. There will be two days of training, a two+ day meeting, and four days of intense collaboration. The meeting features joint & parallel sessions, shared keynotes, poster & demo sessions, birds-of-a-feather, and social events. EDAM, and the tooling around bio.tools for integration with Galaxy, will be presented.

Conference: ELIXIR All-hands (Jun 4-7 2018, Berlin, DE)

https://www.elixir-europe.org/events/elixir-all-hands-2018

The fourth ELIXIR All Hands meeting, bringing together members of the ELIXIR community from across the ELIXIR Nodes, and collaborators from partner organisations, in order to review ELIXIR achievements and activities so far and discuss plans for the future.

Meeting: ELIXIR EXCELERATE WP1 Meeting (Feb 20-22 2018, Copenhagen, DK)

https://tinyurl.com/wp1f2f-2018

A face-to-face meeting to discuss matters around ELIXIR EXCELERATE WP1 (tools) developments. The meeting is primarily for WP1 partners, however anyone who is involved in bio.tools development is welcome to attend.

Workshop: Debian Med 2018 Sprint (Feb 10-12 2018, Barcelona, ES)

https://wiki.debian.org/Sprints/2018/DebianMed2018

This is an informal co-working and co-learning event, participants are welcome to attend on the days that work for their schedule. EDAM and the integration of bio.tools with Debian Med and CWL was worked on.

Meeting: ELIXIR Tools Platform Face to Face Meeting (Feb 8-9 2018, Barcelona, ES)

https://tinyurl.com/etp-feb2018

ELIXIR Tools Platform all-hands meeting to discuss activities of the platform and its projects.

Meeting: ELIXIR EXCELERATE WP2 Meeting (Feb 7 2018, Barcelona, ES)

https://docs.google.com/document/d/1-Ydv-SxTH_aJ4XaGh4g0I1mINgfMKG_yz6wNma1s9hY/edit

Meeting of ELIXIR EXCELERATE WP2 to discuss progress of OpenEBench, strategies for reaching out scientific communities running benchmark activities and practical examples on both technical monitoring and scientific benchmarking activities.

Workshop: bio.tools & EDAM @ 3rd NEUBIAS taggathon (Sep 11-14 2017, Gothenburg, SE)

http://eubias.org/NEUBIAS/what-is-taggathon/new-3-gothenburg-sweden/

The purpose of the taggathons is to implement and feed the content of NEUBIAS webtool; an organized repository of bio image analysis software and workflows for biologists, bioimage analysts and algorithm developers, complementary to ELIXIR bio.tools. The tagathon focuses on curation (identifying and tagging tools), semantics development including synonymous terms between Biology and Image Analysis, with development of EDAM-Bioimaging, and Semantic Web queries.

Conference: ELIXIR Denmark - 3rd Annual Danish Bioinformatics Conference (Aug 24-25 2017, Odense, DK)

http://elixir-node.cbs.dtu.dk/?page_id=2120

The third Danish Bioinformatics Conference organised by ELIXIR Denmark, bringing together members of the bioinformatics community from Denmark and across Europe.

Workshop: ELIXIR-DK / bio.tools Open Day (Aug 23 2017, Odense, DK)

http://tinyurl.com/registryhackathon14

An informal day of presentations, discussion and hacking around activities of the Danish ELIXIR node, including presentations about the ELIXIR Tools and Data Services Registry (https://bio.tools), bio.tools content and feature development, the EDAM ontology, applications of the registry, future plans and more.

Conference: BOSC 2017 (Jul 22-23 2017, Prague, CZ)

The Bioinformatics Open Source Conference (BOSC) is organized by the Open Bioinformatics Foundation (OBF), a non-profit group dedicated to promoting the practice and philosophy of open source software development and open science within the biological research community. BOSC has provided a forum for developers and users to interact and share research results and ideas in open source bioinformatics. EDAM was presented.

Technical hackathon: CodeFest 2017 (Jul 20-21 2017, Prague, CZ)

https://www.open-bio.org/wiki/Codefest_2017

This is an opportunity for anyone interested in open science, biology and programming to meet, discuss and work collaboratively. Everyone is welcome to attend. We will have a mix of experienced developers, newcomers to bioinformatics and everything in between. EDAM and bio.tools integration with the Common Worflow Language (CWL) were worked on.

Conference: ELIXIR All-hands (Mar 20-22 2017, Rome, IT)

https://www.elixir-europe.org/events/elixir-all-hands-2017

The third ELIXIR All Hands meeting, bringing together members of the ELIXIR community from across the ELIXIR Nodes, and collaborators from partner organisations, in order to review ELIXIR achievements and activities so far and discuss plans for the future.

Technical Hackathon: Visual Workflows in bio.tools (Mar 1-3 2017, Tallin, EE)

http://tinyurl.com/registryhackathon13

A three day workshop organised by ELIXIR-EE and partners aiming to implement a proof-of-principle for "visual worfklows" in bio.tools : navigation of bio.tools content with cross-links to TeSS via diagrams for common analytical workflows.

Workshop: The future of proteomics in ELIXIR (Mar 1-2 2017, Tübingen, DE)

https://www.elixir-europe.org/events/strategic-workshop-future-proteomics-elixir

Focussed on creating a white paper to discuss the common infrastructures and services needed by the European proteomics community. bio.tools and EDAM were discussed.

Workshop: ELIXIR discovery portals (ELIXIR Innovation and SME Forum: Genomics and Health - Global resources for local Innovation, Feb 27-28 2017, Helsinki, FI)

The forum was aimed at the companies that use public bioinformatics resources in their business and would like to further streamline this process. The event was jointly organized by ELIXIR Finland, ELIXIR Estonia and the ELIXIR Hub. bio.tools was presented.

https://www.elixir-europe.org/events/elixir-innovation-and-sme-forum%3A-genomics-and-health-global-resources-local-innovation

Meeting: ELIXIR Tools Platform Face to Face Meeting (Feb 22-23 2017, Barcelona, ES)

https://www.elixir-europe.org/events/elixir-tools-platform-all-hands-meeting

The 2nd meeting to discuss progress and plans for the [ELIXIR Tools Platform](https://www.elixir-europe.org/platforms/tools).

Workshop: bio.tools & EDAM @ 2nd NEUBIAS taggathon (Feb 13-15 2017, Oeiras near Lisbon, PT)

http://eubias.org/NEUBIAS/what-is-taggathon/taggathon-2-gulbenkian-oeiras/

The 2nd NEUBIAS Taggathon hosted and supported by the Gulbenkian Institute of Science, organized by the working group "Webtool" (WG4) of NEUBIAS, and in conjunction with the NEUBIAS training school and the following NEUBIAS conference. We extended the bioimaging sub-domain of EDAM in team work with bioimaging experts, and coordinated the development of biii.info/BISE with bio.tools.

Curatathon : Genomics tools in crop & animal breeding (Feb 2-3 2017, Aarhus, DK)

http://tinyurl.com/registryhackathon12

A curation hackathon aimed at curating software tools used for crop and animal breeding research.

Workshop : bio.tools @ Debian Med Sprint (Jan 12-16 2017, Bucharest, RO)

https://wiki.debian.org/Sprints/2017/DebianMed2017

bio.tools folk join the Debian Med folk for co-hacking and co-learning. We improved EDAM annotations in Debian Med, and progressed towards importing high-quality software information from Debian (Med) to bio.tools.

Thematic Hackathon : Computational Proteomics Resources (Jan 10-13, 2017, Semmering, AT)

http://tinyurl.com/registryhackathon11

A thematic hackathon aimed at curating tools for computational proteomics, co-located with the Computational Proteomics Conference.

Technical Hackathon : bio.tools @ NETTAB : (Oct 24 2016, Rome, IT)

http://www.igst.it/nettab/2016/programme/hackathon/

http://tinyurl.com/registryhackathon10

A one day bioinformatics hackathon organized by ELIXIR held in occasion of the NETTAB 2016 Workshop. The hackathon will include the following two main strands: 1) Biosoftware description using bio.tools and schema.org. 2) Deployment of bioinformatics tools and services through Docker.

Workshop: bio.tools & EDAM @ 1st NEUBIAS taggathon (Sep 14-16 2016, Barcelona, ES)

The 1st NEUBIAS Taggathon hosted and supported by Universitat Pompeu Fabra, organized by the working group "Webtool" (WG4) of NEUBIAS, and in conjunction with the NEUBIAS training school. The aim was to bring-in pre-incubated ideas and elements of the next biii.info/BISE webtool and to progress with its implementation. The presence of bio.tools and EDAM projects ensured coordination of NEUBIAS and EuroBioimaging registry and ontology developments with ELIXIR.

http://eubias.org/NEUBIAS/?page_id=228

Conference: ELIXIR-DK @ ECCB (Sep 3-7 2016, The Hague, NL)

http://www.eccb2016.org/

ELIXIR-DK will have a booth at ECCB and will showcase the work of the Danish ELIXIR node including the ELIXIR Tools & Data Services Registry (dev.bio.tools) and the EDAM ontology.

Conference: ELIXIR-DK @ 2nd Annual Danish Bioinformatics Conference (Aug 25-26 2016, Odense, DK)

http://www.conferencemanager.dk/DKBiC-2016/home.html

ELIXIR-DK will have a booth at DKBC and will showcase the work of the Danish ELIXIR node including the ELIXIR Tools & Data Services Registry (dev.bio.tools) and the EDAM ontology.

Workshop : ELIXIR-DK / bio.tools Open Day (Aug 24 2016, Syddansk Universitet, DK)

http://tinyurl.com/registryhackathon9

An informal day of presentations, discussion and hacking, combining two events in one: 1) ELIXIR-DK staff technical get-together and 2) bio.tools workshop.

Conference: ELIXIR-DK @ IMSB 2016 (Jul 8-12 2016, Orlando, USA)

https://www.iscb.org/ismb2016

ELIXIR-DK will have a booth at IMSB 2016 and will showcase the work of the Danish ELIXIR node including the ELIXIR Tools & Data Services Registry (dev.bio.tools) and the EDAM ontology.

Technical Hackathon : Tools, Workflows and Workbenches (May 18-20, 2016, Institut Pasteur, Paris, FR)

http://tinyurl.com/registryhackathon8

A hackathon bringing together developers from key technical projects from ELIXIR and beyond including: the ELIXIR Tools & Data Services Registry (bio.tools), workbench/workflow projects (CWL, Galaxy, Taverna, Arvados), bioinformatics container solutions and registries, and the EDAM ontology.

Resource Hackathon : ELIXIR-SI Tools & Data Services (Apr 8, 2016, University of Ljubljana, SI)

ELIXIR-SI Registry Hackathon will take place on Apr 8, 2016 12-18h at the Faculty of Computer and Information Science (room PR05). The aim of the hackathon is to register Slovenian Bioinformatics Resources and create a national catalogue of Bioinformatics Tools and Data Services.

Thematic Hackathon : Metagenomics Training Resources (Apr 7-8, 2016, EMBL-EBI, UK)

Organised in collaboration with the GOBLET and the ELIXIR Training Platform.

Resource Hackathon : French Tools & Data Services (Mar 24-25, 2016, Gif-sur-Yvette, FR)

http://tinyurl.com/registryhackathon6

A hackathon bringing together representatives of French bioinformatics communities with the ELIXIR Tools & Data Services Registry, dedicated to the description and cataloguing of French tools and services, to boost their discovery and utility.

Resource Hackathon : Norwegian Tools & Data Services (Mar 16-18, 2016, NTNU Trondheim, NO)

A hackathon bringing together representatives of Norwegian bioinformatics communities with the ELIXIR Tools & Data Services Registry, dedicated to the description and cataloguing of Norway tools and services, to boost their discovery and utility.

Resource Hackathon : bio.tools @ Debian Med Sprint (Feb 4-7 2016, Lyngby, DK)

https://wiki.debian.org/Sprints/2016/DebianMed2016

A resource hackathon focussed on curation and software development towards annotation and registration of tool packages from Debian Med. Annotation of Debian Med packages with EDAM.

Resource Hackathon : EMBL EBI tools (Jan 27-28 2016, EMBL EBI, UK)

A mini-hackathon aimed at curation of EMBL EBI software tools.

Resource Hackathon : de.NBI EDAM Codefest (Jan 19-20 2016, Freiburg Uni., DE)

http://tinyurl.com/registryhackathon7

This hackathon, organised by University of Freiburg, will focus on 1) annotation of de.NBI tools and services, 2) ELIXIR Registry and registration process and 3) Publishing tools in the ELIXIR Registry.

Technical Hackathon : EDAM development heuristics (Dec 1-4 2015, Amsterdam, NL)

http://tinyurl.com/registryhackathon5

This hackathon aimed at preparing EDAM for scaling with registry growth. The focus was to enumerate EDAM development heuristics to ensure usability, identify desirable clean-ups, and to devise quality assurance methods, including usability benchmarking in different scenarios. It also included a thematic session focussing on protein structural biology and the WHAT-IF package.

Curatathon : bio.tools curation (Nov 4-6 2015, Brno, CZ)

http://tinyurl.com/registryhackathon3

The second in the series, will aim for representation in the registry of all ELIXIR nodes, including new partners from Spain, Netherlands, Sweden and Finland, and other key resources beyond ELIXIR.

Thematic Hackathon : RNA analysis (Sep 23-25 2015, Copenhagen, DK).

A thematic hackathon focussed on RNA analysis and seeking to establish an ELIXIR RNA Tools Consortium that the Registry can draw upon in the future.

Thematic Hackathon : defining good practice for resource annotation and registry curation (Aug 23-25 2015, Tallin, EE).

http://tinyurl.com/registryhackathon4

A three day workshop organised and financed by ELIXIR-EE aiming to identify relevant processes and good practice for the annotation and curation of resources for their integration into the emerging ELIXIR infrastructure, focussed on next generation sequencing (NGS) analysis and the SeqWIKI Resource Hub.

Technical Hackathon - EDAM Development & Governance (Mar 11-13 2015, Lyngby, DK)

http://tinyurl.com/registryhackathon2

Focused on EDAM technical maintenance and usability, and produced a mock-up of tooling to assure optimal usage of EDAM for registry curation.

Curatathon - Registration of Tool & Data Services (Nov 19-21 2014, Lyngby, DK)

http://tinyurl.com/registryhackathon

Gathered representatives of institutes and key projects within ELIXIR and beyond. The participants performed a valuable pre-release critique of the Registry mechanism and interfaces, and added more than 300 resources to the content.

Mobyle, EDAM and Service Registry hackathon (Jun 17-18 2014, Paris, FR)

Workshop - ELIXIR, BioMedBridges & RDA Workshop: A common vocabulary to classify resources in the life sciences (Oct 7-8 2014, Brussels, NL)

http://www.biomedbridges.eu/news/workshop-common-vocabulary-classify-resources-life-sciences

ALLBIO Workshop - Metagenomics & interoperability (Apr 10-12 2014, Amsterdam, NL)

BioMedBridges AGM Tools Workshop (Mar 9-12 2014, Florence, IT)

bio.tools @ Debian Med Sprint (Jan 31-Feb 3 2014, Aberdeen, UK)

ELIXIR/BioMedBridges Workshop on Tool Registries (Oct 16-18 2013, CBS-DTU, DK)

BioMedBridges Registry Workshop (May 8 2013, Imperial College, UK)

AllBio / EMBRACE Continuity Workshop (Mar 18-20 2013, Amsterdam, NL)

BioMedBridges AGM Registry Workshop (Mar 11-12 2013, Dusseldorf, DE)

EDAM hackathon (Oct 9-13 2012, EMBL-EBI, UK)

AllBio workshop - $\hat{A}_i \hat{A}^\circ$ Web services for improved interoperability in bioinformatics $\hat{A}_i \hat{A}^\pm$ (Oct 2-5 2012, Munich, DE)

14.3 Code of Conduct

We respectfully ask all attendees at meetings to conduct themselves in a way that maintains focus, respect, order - and enjoyment! Suggestions include:

- Bear in mind that you are as responsible for the success of the meeting as anyone else.
- Stick to the meeting agenda if stipulated (most of our meetings do not have rigid agendas).
- Remain focused on the task at hand.
- Come prepared.
- Use an analytic, facts-based approach to problem solving whenever possible.
- Manage meeting time wisely.
- · Brainstorm when fresh ideas are in short supply or complex problems present challenges.
- Allow for the expression of every personÂ;Â⁻s ideas, and give all ideas a serious hearing.
- Listen carefully to each other, and be courteous.
- · Accommodate disagreements and criticisms without hostility.
- Refrain from all personal attacks.
- Demonstrate flexibility.
- Make meetings enjoyable; employ humour and respect.
- Resolve conflict through compromise and consensus whenever possible.

Governance

bio.tools follows a simple governance model of three tiers under the leadership of the Danish ELIXIR node (Professor Søren Brunak, Head of Node) which is providing long-term funding and support for *bio.tools*. Development on the ground is led by Danish Node staff, currently Jon Ison, Piotr Chmura and Hans Ienasescu, in close collaboration with the registry-dev group (see below) and EDAM developers.

If you'd like to get involved with the project please mail registry@elixir-dk.org.

15.1 registry-dev

registry-dev includes the technical and scientific experts at the heart of the development and curation of *bio.tools*. Priorities are set in a quasi-democratic way; *bio.tools* is a "do-ocroacy" with the Danish ELIXIR Node staff having the final say, where necessary (in so far as this is meaningful). registry-dev members are either funded, or have the intent and some bandwidth, to support *bio.tools* in the long-term. Danish Node staff ensure the registry-dev group and all Contributors are listened to and informed.

Members of registry-dev are responsible for agreeing aims and general good practice. They are expected to advocate *bio.tools* and (as bandwidth allows) collaborate with one another to help develop the registry software, related technical projects and registry content, *e.g.*:

- add new and improve existing content through collaboration with EDAM Developers
- · routine content maintenance including quality control
- work collaboratively within the Curation Task Force (see below) and attend Hackathons
- suggest or implement new features
- · develop software for the registry and related technical projects
- · evaluate the registry and provide feedback, to ensure the registry software is fit for purpose

Danish Node staff are responsible for reporting software development and curation priorities, and progress, to the ELIXIR-DK Management.

registry-dev will assemble virtually or in person as circumstances dictate, in meetings with open agenda and followed up with actions and notes on key recommendations. registry-dev members are signed up to the the registry-core mailing list.

15.1.1 Thematic editors

Named **thematic editors** are registry-dev members responsible for overseeing coverage and quality in specific thematic areas, *e.g.*

- evaluating existing coverage (EDAM, tools)
- driving coverage (EDAM, tools)
- · liasing with community & leading workshops in their specialist area

See the Editors Guide.

15.2 Registry contributors

Registry contributors include anyone who makes significant contributions to the registry content or registry-related software, by whatever means, but have none of the responsibilities or expectations of registry-dev.

An important (but voluntary) role of contributors is to function in an **advisory capacity**, *i.e.* review the progress and priorities of registry-dev and advise them on their priorities and how best to achieve the current aims. To these ends, the following actions are welcome: - read the *bio.tools* milestones and changelog and provide feedback on the reported progress and priorities. - oversee the curation and development of *bio.tools* and actively offer constructive advice based on their practical experience, requirements and expertise - advocate *bio.tools* to colleagues

The registry-dev group will respect this feedback and advice and reflect it in subsequent rounds of development and curation. We very much welcome new contributors: for further information please mail registry@elixir-dk.org.

15.3 Registry end-users

We particularly welcome input from end-users from the life science community including scientists, technicians and managers from academia and industry: - to test, evaluate and critique the registry software and content - to provide feedback and constructive advice based on their practical experience, requirements and expertise

registry-dev will respect this feedback and advice and reflect it in subsequent rounds of registry development and curation. Anyone who is considering using the registry - but especially typical scientist / bioinformatician end-users - are welcome to mail registry@elixir-dk.org.

Contributors

Note: You can contact the registry-dev group by mailing registry-core@elixir-dk.org

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16.4 Registry Contributors

Thanks to the many people who have contributed - if you're not listed below, please let us know!

• Aleksandra Nenadic (University of Manchester)

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Code

Note: We are in the process of packaging the system in a docker container to achieve a more reproducible, environment-independent local deployment solution. In the meantime please see our guidelines below which summarie necessary components and steps to run *bio.tools*.

17.1 Source code

The source code of the registry is under standard GPL 3.0 license and is available from https://github.com/bio-tools/ biotoolsRegistry/.

17.2 Architecture

The architecture of the registry is designed around the principle of decoupling frontend from the backend in order to eliminate performance bottlenecks at scale. The backend serves the data through the RESTful APIs which are in turn consumed by the the frontend SPA (Single-Page Application). The main advantage of this paradigm is that the frontend uses the exact same API calls that any user can invoke in order to create their own customized interface. The overall goal of scalability can be achieved by hosting the components independently (master database, replicated cache layer and static frontend code in a CDN - Content Delivery Network - such as Cloudflare or Akamai).

17.3 Components

You only need Docker to run bio.tools locally.

Installing bio.tools on your system

The local (development) installation is done via Docker. Other than Git (and a text editor), nothing else is required to run and write code for bio.tools.

18.1 1. Download and Install Docker

18.1.1 Docker main installation page

https://docs.docker.com/install/

Note: You will need to create a Docker Hub account.

Windows

https://docs.docker.com/docker-for-windows/install/

Note: Read the "What to know before you install" information to see if Docker Destktop for Windows can be installed on your system. If your system does not meet the requirements to run Docker Desktop for Windows, you can install the legacy Docker Toolbox.

MacOS

https://docs.docker.com/docker-for-mac/install/

CentOS

https://docs.docker.com/install/linux/docker-ce/centos/

Debian

https://docs.docker.com/install/linux/docker-ce/debian/

Fedora

https://docs.docker.com/install/linux/docker-ce/fedora/

Ubuntu

https://docs.docker.com/install/linux/docker-ce/ubuntu/

18.2 2. Clone the repo

18.2.1 Using HTTPS

git clone https://github.com/bio-tools/biotoolsRegistry.git

18.2.2 Using SSH

git clone git@github.com:bio-tools/biotoolsRegistry.git

Go into the folder in which you cloned the bio.tools repo. By default it will be called biotoolsRegistry: (e.g. cd biotoolsRegistry or cd /home/user/coding/biotoolsRegistry)

18.2.3 3.0 Inside the bio.tools repo

Note: The Docker setup will require up to 5 GB of disk space. The bio.tools data will also add to this.

18.2.4 3.0.1 Build the necessary Docker images

```
docker-compose build
```

The above command will download / build all the Docker images required for bio.tools to run on your local machine.

The images built can be seen by running: docker image 1s and are:

- biotools/frontend (~ 827MB)
- biotools/backend (~ 1.12GB)
- mysql (~ 205MB) (will show up after running 3.0.2)
- elasticsearch (~ 486MB) (will show up after running 3.0.2)
- python (~ 925MB)
- node (~ 650MB)

18.2.5 3.0.2 Create and run the Docker containers

docker-compose up

The above command will create and run the required containers:

• biotools-mysql

- biotools-elasticsearch
- biotools-backend (depends on biotools-mysql and biotools-elasticsearch)
- biotools-frontend (depends on biotools-backend)

Note: After running the docker-compose up command, the containers will start and will output log messages which you can see in your terminal window. In order for the containers to keep running this window needs to stay open. You will need to open new terminal windows/tabs for other operations.

docker-compose up will also build the images if they do not exist, but in order to be sure your latest source code and image changes are running make sure you run docker-compose build beforehand

Too see the running containers run: docker container ls

18.3 3.1 The short(er) setup

Run the steps below in the root folder of the Git project (e.g. biotoolsRegistry)

18.3.1 3.1.1 Make migrations

docker exec biotools-backend python manage.py makemigrations

Make Django migrations from the exiting models. Executed on the biotools-backend container. If you get the No changes detected message it means that you are up to date.

18.3.2 3.1.2 Migrate to the DB

docker exec biotools-backend python manage.py migrate

Create necessary tables and other DB objects from the migrations. Executed on the biotools-backend container. If you get the No migrations to apply. message it means that you are up to date.

18.3.3 3.1.3 Copy initial (seed) DB

docker cp initial_db.sql biotools-mysql:/root

Copies the initial_db.sql SQL file into the biotools-mysql container (where the MySQL database server runs) into the /root folder.

18.3.4 3.1.4 Copy initial DB load script file

docker cp load_initial_db.sh biotools-mysql:/root

Copies the load_initial_db.sh into the biotools-mysql container. This file will run the MySQL commands used to load the database described in initial_db.sql

18.3.5 3.1.5 Execute initial DB load script file

docker exec biotools-mysql bash /root/load_initial_db.sh

Executes the load_initial_db.sh file in the biotools-mysql container which loads the initial (seed) DB data.

Note: The initial DB contains 11 tool annotations, a superuser (username: biotools, password: biotools), an initial test subdomain and the necessary EDAM files. See 3.1.8 for more.

18.3.6 3.1.6 Purge Elasticsearch

docker exec biotools-backend python manage.py es_purge

Purges (clears) any data in the Elasticsearch index. Executed in the biotools-backend container which communicates with the biotools-elasticsearch container.

18.3.7 3.1.7 Regenerate Elasticsearch

docker exec biotools-backend python manage.py es_regenerate

Takes all the tools, subdomains annotations etc. in the DB and creates the equivalent entries in the Elasticsearch index. Executed in the biotools-backend container.

18.3.8 3.1.8 Done

At this point you can go to http://localhost:8000 to see the local bio.tools homepage.

The test subdomain can be viewed at http://test.localhost:8000

You can login with the existing superuser (user: biotools, password: biotools).

All running Docker containers can be stopped by running: docker-compose down from the root Git folder. This will preserve the data in the MySQL database and Elasticsearch. To reinstantiate everything again run: docker-compose up.

Only need to run docker-compose build once at the beginning or if changes are made to the bio.tools Docker settings files.

If you wish to remove the data along with the containers run: docker-compose down -v which will also remove the Docker volumes which preserve the MySQL and Elasticsearch data.

18.4 3.2 The longer setup

This is an alternative to **3.1** in which some of the steps were contained in the initial DB files. This will start with no data.

Run the steps below in the root folder of the Git project (e.g. biotoolsRegistry)

18.4.1 3.2.1 Make migrations

docker exec biotools-backend python manage.py makemigrations

Make Django migrations from the exiting models. Executed on the biotools-backend container.

18.4.2 3.2.2 Migrate to the DB

docker exec biotools-backend python manage.py migrate

Create necessary tables and other DB objects from the migrations. Executed on the biotools-backend container.

18.4.3 3.2.3 Create a superuser

docker exec -it biotools-backend python manage.py createsuperuser

Prompts the creation of a superuser, need to input superuser name, email (optional) and password. Executed on the biotools-backend container.

18.4.4 3.2.4 Setup EDAM ontology

docker exec biotools-backend bash /elixir/application/backend/data/edam/update_edam.sh

Download EDAM ontology and push it to the DB. Can also be used to update to new EDAM version. The file which indicates the EDAM version is <git_project_root>/backend/data/edam/current_version.txt, e.g. biotoolsRegistry/backend/data/edam/current_version.txt

18.4.5 3.2.5 Copy helper tables SQL

docker cp update_site_settings.sql biotools-mysql:/root

Copies the update_site_settings.sql SQL file into the biotools-mysql container (where the MySQL database server runs) into the /root folder. This file contains SQL instructions used to create helper tables and settings for the project.

18.4.6 3.2.6 Copy script file to run helper tables

docker cp update_site_settings.sh biotools-mysql:/root

Copies the update_site_settings.sh into the biotools-mysql container. This file will run the MySQL commands described in update_site_settings.sql

18.4.7 3.2.7 Execute script file

docker exec biotools-mysql bash /root/update_site_settings.sh

Executes the update_site_settings.sh file in the biotools-mysql container which loads the helper tables and settings in the DB.

18.4.8 3.2.8 Purge Elasticsearch

docker exec biotools-backend python manage.py es_purge

Purges (clears) any data in the Elasticsearch index. Executed in the biotools-backend container which communicates with the biotools-elasticsearch container.

18.4.9 3.2.9 Regenerate Elasticsearch

docker exec biotools-backend python manage.py es_regenerate

Takes all the tools, subdomains annotations etc. in the DB and creates the equivalent entries in the Elasticsearch index. Executed in the biotools-backend container.

18.4.10 3.1.10 Done

At this point you can go to http://localhost:8000 to see the local bio.tools homepage.

Login with the user created in 3.2.3

No tools or subdomains are available, add tools at http://localhost:8000/register and subdomains at http://localhost: 8000/subdomain

All running Docker containers can be stopped by running: docker-compose down from the root Git folder. This will preserve the data in the MySQL database and Elasticsearch. To reinstantiate everything again run: docker-compose up.

Only need to run docker-compose build once at the beginning or if changes are made to the bio.tools Docker settings files.

If you wish to remove the data along with the containers run: docker-compose down -v which will also remove the Docker volumes which preserve the MySQL and Elasticsearch data.

18.5 4. Useful information

18.6 4.0 Basic usage

After completing steps 1-3 above, the only required commands for basic use are

docker-compose up

and

docker-compose down

and perhaps

docker-compose down -v

18.7 4.1 Local dev

After running docker-compose up you will see a number of log messages. These messages come from the running containers:

- biotools-mysql (MySQL logs)
- *biotools-elasticsearch* (Elasticsearch logs)
- *biotools-backend* (Mostly Apache logs, sometimes Python logs)
- *biotools-frontend* (Gulp logs)

18.7.1 4.1.1 Backend dev

The biotools-backend container is based on an image which uses an Apache server. The logs from biotools-backend come from Apache or sometimes from Python.

Note: Changes in Python/Django/backend files will be reflected in the biotools-backend container, **BUT** because of how Apache works, the changes won't be reflected in your browser http://localhost:8000 until Apache is reloaded. In order to see the changes in the reflected in the browser you need to run:

docker exec biotools-backend /etc/init.d/apache2 reload

Remember to run the above command whenever you want to see your code changes reflected in your local bio.tools.

Bringing the containers down and up agail will also work, but this takes significantly longer. The above command is almost instant.

Most issues with the backend code will be reflected in the browser at http://localhost:8000/api/ {some_path}, e.g. http://localhost:8000/api/tool or http://localhost:8000/api/jaspar etc.

See https://biotools.readthedocs.io/en/latest/api_reference.html or Django route files (urls.py) for more API end-points.

18.7.2 4.1.2 Frontend dev

The biotools-frontend container outputs logs from gulp (https://gulpjs.com/) which bundles all frontend JavaScript and CSS code.

Every time you change and save a .js or .css file in the frontend, gulp will re-bundle everything automatically. This implies that all changes in the frontend are reflected automatically in thr browser, unlike for the backend.

Note: If you have a syntax error in your JavaScript or CSS files, gulp will fail and you won't see any changes reflected in the browser. So, if your changes are not reflected, look at the biotools-frontend logs of gulp which will indicate if you made a syntax error in your code.

18.8 4.2 Update EDAM

Similarly to section **3.2.4**, in order to update to the latest EDAM version (or just use a different EDAM version) the update_edam.sh needs to be executed on the biotools-backend container.

The version number used for updating EDAM is specified in the file:

<pit_project_root>/backend/data/edam/current_version.txt

In order to update to the latest EDAM version (e.g. 1.23) edit the current_version.txt file to store the value 1.23, save the file and run:

docker exec biotools-backend bash /elixir/application/backend/data/edam/update_edam.sh

The script file will download the specific EDAM version .owl file from https://github.com/edamontology/ edamontology and execute the:

python /elixi/application/manage.py parse_edam

command in the biotools-backend container.

Note: The current_version.txt file is tracked by Git and any changes involving EDAM versions other than latest should not be pushed to the main branches of the repo.

18.9 4.3 Local email setup

Important to note that the email system used to send emails regarding account creation and password reset will not work as intended out of the box .

In order for the emails to work you need to provide credetials (email, password, smtp settings) in the backend/ elixirapp/settings.py file. bio.tools production uses Zoho mail (http://zoho.com) which currently works well with our setup.

The easy way would be to make a Zoho email account and use that email information to make the email functionality run. Gmail and Yahoo were tried and the connections are blocked by Gmail and Yahoo because of security reasons. This is because Gmail and Yahoo don't accept a simple username-password login and require more strict settings. Feel free to implement this in your bio.tools instance.

18.10 4.4 Docker notes

18.10.1 Build bio.tools Docker images

docker-compose build

18.10.2 Run bio.tools containers

docker-compose up

18.10.3 Stop bio.tools containers

docker-compose down

18.10.4 Stop bio.tools containers and remove data

docker-compose down -v

18.10.5 View running containers

docker container ls

18.10.6 View all containers

docker container ls -a

18.10.7 Remove stopped containers

docker container rm <CONTAINER_ID>

or

docker container rm <CONTAINER_ID1> <CONTAINER_ID2> <CONTAINER_ID3>

18.10.8 Force remove containers

```
docker container rm -f <CONTAINER_ID>
```

or

docker container rm -f <CONTAINER_ID1> <CONTAINER_ID2> <CONTAINER_ID3>

18.10.9 Prune containers (Remove all stopped containers)

docker container prune

18.10.10 View images

docker image ls

18.10.11 Remove image

docker image rm <IMAGE_ID>

or

docker image rm <IMAGE_ID1> <IMAGE_ID2> <IMAGE_ID2>

(will not work if containers are running this image)

18.10.12 Enter a container and run commands

Any of the bio.tools running containers can provide a bash terminal to run commands inside the containers (similar to docker exec). Examples of the commands are:

```
docker exec -it biotools-mysql bash
docker exec -it biotools-elasticsearch bash
docker exec -it biotools-backend bash
docker exec -it biotools-frontend bash
```

As an example, to view the info in a MySQL database table run:

- 1. docker exec -it biotools-mysql bash
- 2. In container: mysql -u elixir -p (password is by default 123)
- 3. In MySQL:

```
use elixir;
SELECT * FROM elixir_resource WHERE visibility = 1;
```

18.10.13 bio.tools Docker settings files:

Backend build config file

<git_project_root>/backend/Dockerfile

Backend dockerignore file

<git_project_root>/backend/.dockerignore

Frontend build config file

<pit_project_root>/frontend/Dockerfile

docker-compose YAML config file

<pit_project_root>/docker-compose.yml

18.10.14 Docker documentation:

- https://docs.docker.com/
- https://docs.docker.com/reference/
- https://docs.docker.com/engine/reference/commandline/container/
- https://docs.docker.com/engine/reference/commandline/image/
- https://docs.docker.com/config/pruning/

- https://docs.docker.com/compose/
- https://hub.docker.com/

18.11 API Guidelines

You can also check out our API instructions at the links below:

- API reference
- API Usage Guide

License

The registry content is freely available to all under the Creative Commons Attribution licence (CC BY 4.0). The source code of the registry is under standard GPL 3.0 license.

Publications

Ison, J. et al. (2019). The bio.tools registry of software tools and data resources for the life sciences. Genome Biology, doi:10.1186/s13059-019-1772-6

Ison, J. et al. (2019). Community curation of bioinformatics software and data resources. Briefings in Bioinformatics. doi:10.1093/bib/bbz075

Tsiamis, V. et al. (2019) A Thousand and One Software for Proteomics: Tales of the Toolmakers of Science. Journal of Proteome Research. doi:10.1021/acs.jproteome.9b00219

Palmblad, M., Lamprecht, A-L, Ison, J. and Schwammle, V. (2018) Automated workflow composition in mass spectrometry based proteomics *Bioinformatics* doi:10.1093/bioinformatics/bty646

Hillion K.H., Kuzmin I., Khodak A., Rasche E., Crusoe M., Peterson H., Ison J., Ménager, H. (2017). Using bio.tools to generate and annotate workbench tool descriptions *F1000Research* (article). doi:10.12688/f1000research.12974.1

Doppelt-Azeroual, O., Mareuil, F., Deveaud, Kalaš, M., Soranzo, N., van den Beek, M., Grüning, B., Ison, J. and Ménager, H. (2017). ReGaTE: Registration of Galaxy Tools in Elixir *GigaScience*, doi:10.1093/gigascience/gix022

Ménager, H., Kalaš, M., Rapacki, K. and Ison, J. (2016). Using registries to integrate bioinformatics tools and services into workbench environments *Int J Softw Tools Technol Transfer*, doi:10.1007/s10009-015-0392-z

Ison, J. et al. (2015). Tools and data services registry: a community effort to document bioinformatics resources. *Nucleic Acids Research*, doi: 10.1093/nar/gkv1116

Ison, J., Kalaš, M., Jonassen, I., Bolser, D., Uludag, M., McWilliam, H., Malone, J., Lopez, R., Pettifer, S. and Rice, P. (2013). EDAM: an ontology of bioinformatics operations, types of data and identifiers, topics and formats *Bioinformatics*, doi: 10.1093/bioinformatics/btt113

20.1 Citation

If you use bio.tools, please cite:

Ison, J. et al. (2015). Tools and data services registry: a community effort to document bioinformatics resources. *Nucleic Acids Research.* doi: 10.1093/nar/gkv1116

If you use EDAM or its part, please cite:

Ison, J., Kalaš, M., Jonassen, I., Bolser, D., Uludag, M., McWilliam, H., Malone, J., Lopez, R., Pettifer, S. and Rice, P. (2013). EDAM: an ontology of bioinformatics operations, types of data and identifiers, topics and formats *Bioinformatics*, doi: 10.1093/bioinformatics/btt113

Support

For help, support and feedback, please mail registry-support.

These docs

Note: Help with these docs is greatly appreciated. You can work on them directly via GitHub or make comments, requests, report bugs *etc* by using the issue tracker.

Documentation for bio.tools and related projects are maintained in GitHub:

https://github.com/bio-tools/biotoolsDocs

Documentation files are written in **reStructuredText** and have the file extension .rst. Uploading a file to GitHub will trigger a rebuild of the docs. GitHub include the file index.rst which defines the menu structure. Each menu item corresponds to a GitHub file, which (by convention) should have the same name as the menu item: use concise names!

22.1 reStructuredText links

- rST and Sphinx CheatSheet
- Quick Reference
- Primer
- Full documentation
- Online editor
- readthedocs FAQ
- readthedocs : getting started
- readthedocs build process
- thread on wide table handling
- links in rst docs