One Thousand and One Software for Proteomics

Tales of the Toolmakers of Science

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Article

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A Thousand and One Software for Proteomics: Tales of the Toolmakers of Science

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Abstract

Proteomics is a very active field driven by frequent introduction of new technological approaches, leading to high demand for new software tools and the concurrent development of many methods for data analysis, processing and storage. The rapidly changing landscape of proteomics software makes finding a tool fit for a particular purpose a significant challenge. The comparison of software and the selection of tools capable to perform a certain operation on a given type of data relies on their detailed annotation using well-defined descriptors. However, finding accurate information including tool input/output capabilities can be challenging and often heavily depends on manual curation efforts. This is further hampered by a rather low half-life of most of the tools, thus demanding the maintenance of a resource with updated information about the tools. We present here our approach to curate a collection of 189 software tools with detailed information about their functional capabilities. We furthermore describe our efforts to reach out to the proteomics community for their engagement, which further increased the catalogue to >750 tools being about 70% of the estimated number of 1,097 tools existing for proteomics data analysis.

Descriptions of all annotated tools are available through https://proteomics.bio.tools

Keywords: Catalogue, community, software tools, curation, data analysis, collection, annotations, developers, registry, descriptions

Introduction

Proteomics is a dynamic field. New experimental procedures continually emerge, driving the development of new analytical methods and software tools, and the adaptation of existing methods and tools for new types of data. Over the last two decades, hundreds of academic groups and individual researchers have produced, we estimate (see *Sources of information* below), some 75,000 publications and at least 1000 software tools, servicing a far smaller number of common operations in proteomics data analysis. While this great wealth is welcome, it presents the scholar with significant challenges to find, compare and select appropriate tools for the problem at hand, giving rise to various attempts to describe, organise and present the available offerings.

In the early 1990s, a manually curated Gopher or Web link collection was the place to find and share information about online services in a particular domain. For bioinformatics there was "Pedro's BioMolecular Research Tools", a list of software and databases maintained by Dr. Pedro M. Coutinho, until he graduated from Iowa State University in December 1996. "Pedro's List" went permanently off-line sometime in late 2006 or early 2007, but inspired many other efforts in its wake. [1,2] For example, the ms-utils.org wiki (https://ms-utils.org) was created by M. Palmblad in 2006 to collect and curate free (gratis) software for analysis of mass spectrometry data in proteomics. It includes a variety of useful information, including supported data formats, programming language, and links to source code. Tools are sorted into categories such as peak picking, protein quantitation and mass spectrometry imaging, and subcategories where needed. ms-utils.org is manually curated by a community effort, including many of the software authors, and currently (Mar 2019) contains 244 annotated tools and 141 literature references,

But what about Pedro's biomolecular research tools? How many are still available at their original location? Not many, as it turns out. Of the 184 tools (excluding mirrors) listed in the "Part 1: Molecular Biology Search and Analysis" of Pedro's list (last updated June 15, 1996) only 6 (or 3%) could be found at their original URL 23 years later, suggesting a tool *URL* half-life of approximately 4.7 years; a link rot of 14% per year. If one discounts the 11 listed Gopher or 5 FTP resources (none still available in March 2019), and 6 tools which could be located by

URL redirection, the half-life is 6.0 years, assuming exponential decay. The services that are still findable include several on ExPASy [3] maintained by the Swiss Institute of Bioinformatics. PredictProtein [4], one of the first Internet servers in molecular biology, is still available, albeit through an automatic redirection since it was relocated in 2013 (after 21 years of service). However, these conscientiously maintained tools are rare exceptions. Things are more heartening in the case of mass spectrometry-based proteomics. We extracted 55 publications describing at least one new software tool (excluding databases and tool reviews) by searching PubMed for "mass spectrometry" and “software” in the title, abstract or full text from 2000, 2005, 2010 and 2015. Two out of five tools from 2000 were still available in 2019 (one more replaced by a tool with a different name), as were 3/7 from 2005, 6/10 from 2010 and 29/33 of the tools published in 2015. This gives a tool half-life of around 12 years, twice that for Pedro’s list. This may be explained in part by mass spectrometry still being used in similar ways as in the late 1990s, whereas genome sequencing methods have changed dramatically, making older tools obsolete.

Clearly, there is an enduring requirement for ways to describe and catalogue tools, to ensure the legacy of development is not lost, and in turn, promote the repurposing of tools to avoid reinvention. It is precisely this need that motivates the *bio.tools* initiative [5] to provide, under a convenient portal (https://bio.tools), a registry of standardised information for over 12,000 bioinformatics tools, providing end-users a convenient means to find, understand, compare and select appropriate tools for their research. New software tools, web applications and databases for proteomics constantly appear, and the recently published[5,6] first Special Issue of the *Journal of Proteome Research* [5,6] provides an accessible resource of tools selected for their applicability and ease of adoption. Here we describe an effort (Figure 1) where the ms-utils.org and *bio.tools* developers have joined forces, to strive for high quality descriptions and comprehensive coverage of the prevalent proteomics research software. We describe our curation method and summarise the 754 annotated proteomics tools currently available in *bio.tools*. The work is assisted by the fledgling Proteomics Community [7] under the auspices of ELIXIR, the European Infrastructure for Biological Information. The latter organization will provide ongoing support as part of its infrastructure to ensure *bio.tools* content will continuously be updated and the service further improved. The process is community-driven and we invite and welcome the broader proteomics community to participate.

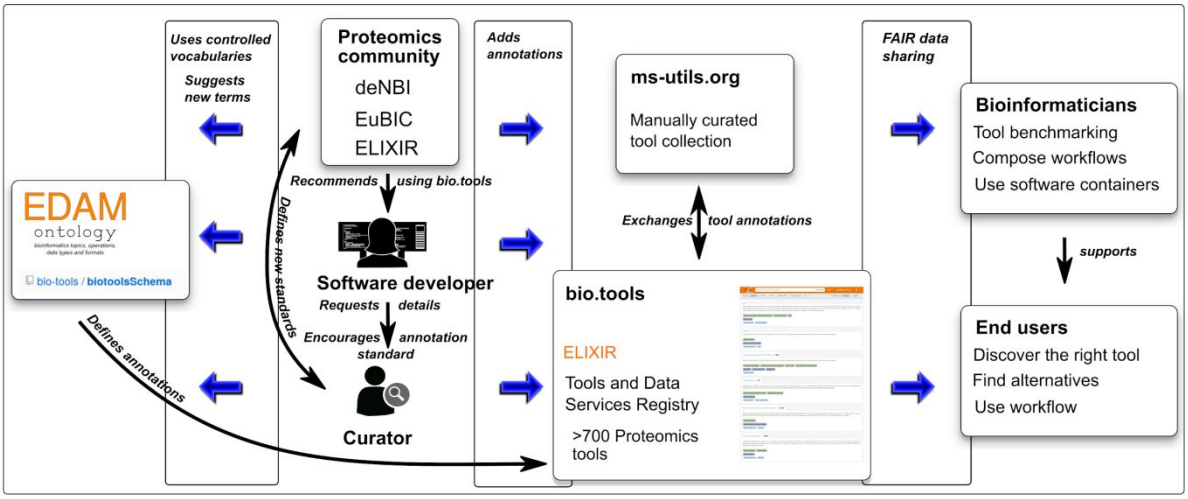

Figure 1. The relationships between the EDAM ontology, *bio.tools*, ms-utils.org, the proteomics community and tool curators.

Methods

Software descriptors

biotoolsSchema (https://github.com/bio-tools/biotoolsschema) defines a controlled vocabulary and precise syntax for some 50 general software attributes such as name, description, software license and programming language. *bio.tools* uses a simplified model of software, defined by biotoolsSchema, where a tool (Figure 2) can have one or more basic functions or modalities, each expressed in terms of input and output data types, specific operations and supported data formats. The schema was recently extended to allow the annotation of tool relationships, for example single-operation tools being part of a multi-functional software suite.

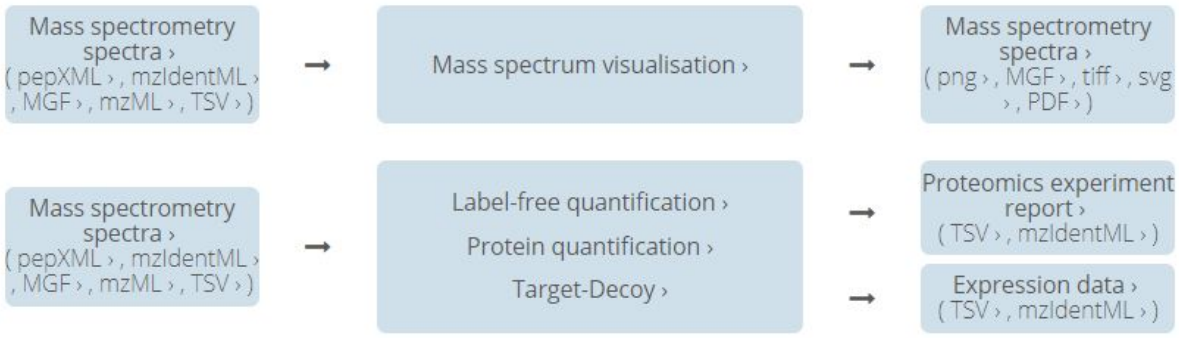

Figure 2. Extract from *bio.tools* Tool Card for PeptideShaker (https://bio.tools/peptide-shaker) summarising the tool's basic functionality. The tool has two major modes. The figure includes types of data and supported data formats for input (left of figure) and output (right), and specific operations performed (centre).

When describing a tool, it's necessary to identify the distinct functions and the individual operations, inputs and outputs (including types of data and supported formats) associated with each one. These attributes are covered by the **EDAM ontology** [7,8] (http://edamontology.org) which provides a precise nomenclature for scientific characterisation of tools, including *topic* (a category within the life sciences, *e.g.* "Proteomics"), *operation* (*e.g.* "Peptide identification"), *data* (*e.g.* "Mass spectrometry spectra") and *format* (*e.g.* "Thermo RAW"). Finally, an emerging information standard (https://bio-tools.github.io/Tool-Information-Standard/) used by *bio.tools* defines 5 tiers (from "Sparse" to "Comprehensive") of progressively richer annotation that may be provided for a tool. For example, the "Basic details" tier mandates annotations for tool name, description, homepage, unique ID, tool type, scientific topic, publication and support (contact) information.

Sources of information

A search in PubMed for publications throughout the last two decades returns 76,689 hits for the search term "proteomics", and 1,097 hits for the query ("new software" OR "new algorithm" OR "new web service" OR "novel software" OR "novel algorithm" OR "novel web service") AND "proteomics" - giving a reasonable estimate of the number of proteomics publications and software tools. Thus, there is a wealth of information that can be mined when producing tool descriptions. When registering tools in *bio.tools*, we used various sources of information, listed below in approximate order of priority when annotating a tool:

1. existing annotations in ms-utils.org
2. the primary publication about the tool
3. the official website of the tool and/or online repository in cases of open source tools
4. official documentation
5. other text materials, *e.g.* publications demonstrating tool usage, supplementary files, tutorials *etc.*
6. source code and testing of software functionality after installation

Particular attention was made of passages and sentences that are highly descriptive of the tool's functionality as these were used later, when identifying relevant EDAM terms.

Registration of software information

Anyone with a *bio.tools* account can add new entries, or edit existing entries subject to edit rights which are shareable between users. *bio.tools* supports manual registration via the *bio.tools* registration user interface, and registration via API by submission of a file in JSON or XML format, which must conform to biotoolsSchema. The ms-utils.org wiki has been built up over more than a decade by several contributors adding new tools as they appear or were discovered in the literature. Defunct but historically important tools are kept in the list, though dead links are removed, distinguishing these tools from those still available. The annotations are all done manually by editing the wiki page directly, requiring basic familiarity with the wiki format.

Curation process

We sought to optimize the curation of proteomics tools by producing high-quality annotations on a subset of 189 tools from the full proteomics collection. The curation of this corpus of proteomics tools involved a multi-step process:

1. *Compile list of proteomics resources.* We took as a starting point what was available in ms-utils.org and *bio.tools*, augmenting this with lists of tools harvested from Web searches and by searching the scientific literature. The tool name, homepage URL and publication DOI (where available) were recorded: for convenient co-editing a shared spreadsheet was used, which included, for later use, controlled vocabularies (from EDAM and biotoolsSchema) for attributes of interest.
2. *Establish curation priorities.* Our main priority was to provide information corresponding to the "Detailed" tier from the Tool Information Standard for every tool: tool name, description, homepage, tool type, scientific topic, publication (DOI), support information (a link to a helpdesk, issue tracker or mailing list, or an email or URL for a contact person), scientific operation, documentation (URL), operating system, programming language and license. A secondary priority was to annotate the data formats supported by tools.
3. *First curation pass*. We recorded whatever attributes were immediately obvious from superficial inspection of the tool publication and homepage, typically not spending more than 10 minutes per tool.

Where EDAM annotations could not immediately be assigned, passages or sentences describing the tool functionality were recorded, to be used later as a source of key words for assignment or creation of new EDAM topic, operation, data or format terms.

4. *Further curation passes*. We recorded attributes from a deeper inspection of the tool materials, progressively enriching the metadata according to tiers from the Tool Information Standard. Various browsers and utilities (Table 1) were used to make EDAM annotations, noting any new required terms. To provide reliable, consensus annotations, tools were independently annotated and annotations cross-validated, recording any disagreements that warranted further investigation.
5. *Refinement of EDAM annotations and ontology.* We inspected EDAM annotations across the corpus of tools, making adjustments where necessary to ensure consistency and finalise a definite list of new terms. EDAM was extended with the new concepts (terms), synonyms of existing concepts and various other changes to improve the concept hierarchy and usability.
6. *Update of ms-utils.org and bio.tools*. The spreadsheet was transformed to biotoolsSchema-compatible XML, the data validated against the biotoolsSchema and uploaded to *bio.tools* via API. In some cases, where pre-existing entries were not owned by us, the new data was carefully merged into the existing records. Some entries were subsequently polished using the the *bio.tools* registration interface. ms-utils.org was updated with new information and entries by manual editing. Links were added, from *bio.tools* to ms-utils.org for every tool listed in both resources, and from ms-utils.org subject categories to EDAM, where possible.

Utility	**Description**	**URL**
OLS	Ontology Lookup Service from EMBL-EBI	www.ebi.ac.uk/ols/ontologies/edam
BioPortal	Ontology browser from NCBO	bioportal.bioontology.org/ontologies/EDAM
EDAM Browser	EDAM ontology browser from IFB	ifb-elixirfr.github.io/edam-browser
EDAM Annotator	Emerging utility for annotating tools using EDAM	people.binf.ku.dk/vzn529/eta
EDAM Map	Utility for mapping text (terms, phrases and free text) to EDAM	biit.cs.ut.ee/edammap

Table 1. Browsers and utilities that are useful when annotating software tools

Community engagement

The work built upon lists of tools, preliminary EDAM terms and annotations provided by contributors to ms-utils.org, independent editors of *bio.tools* for example from the de.NBI infrastructure (https://www.denbi.de/), and by participants at a hackathon of the EuBIC Winter School 2017 .[9] This "long tail" of contribution from the proteomics research and tool user community presented an invaluable starting point for the work. The bulk of subsequent curation work was achieved through a *bio.tools* studentship (http://biotools.readthedocs.io/en/latest/studentships.html); a scheme run by the Danish ELIXIR node to support early career stage scholars to contribute to *bio.tools* and gain experience with the ELIXIR infrastructure. Following broad ranging discussions, we distilled two primary goals. First, the entire tools corpus should be collated and described in at least a basic level of detail. Second, for a subset of high priority tools, the annotations should enable the construction of data analysis workflows, which implies a greater level of detail including supported data formats. The work is in context, and but a small part of, a broader sweep of action in scope of the emerging ELIXIR Proteomics Community (https://www.elixir-europe.org/communities/proteomics) including data integration with other omics data, automatized data processing and standardization including the description of software in *bio.tools*.

Results and discussion

bio.tools includes a total of 754 tools with the EDAM Topic annotation of "Proteomics" (EDAM:topic_0121), "Proteomics experiment" (EDAM:topic_3520), or synonyms of these terms. These tools are, for convenience, associated with a *bio.tools* subdomain available for browsing at https://proteomics.bio.tools. The tool descriptions include a total of 30,187 annotations, of which 6,350 are EDAM annotations. The metadata richness of these tools (Table 2) according to the Tool Information Standard shows that 81% of the collection have "Detailed" (or richer) annotation. Of this corpus, this work contributed 189 new tool registrations in *bio.tools*, of which 167 are annotated to at least "Detailed" level. Of these 189 tools, 93% (176) have an input or output defined, with a total of 562 EDAM Data annotations and 963 EDAM Format annotations. The corpus of 754 tools includes command-line tools (276, 31%), web applications (224, 25%), desktop applications (170, 19%), libraries (97, 11%) and a long tail of other tool types defined in biotoolsSchema (note that a single tool can be annotated

as of more than one basic type). The ms-utils.org wiki has been structured according to the EDAM ontology, linking most tool categories to EDAM operations. As a single-page wiki, a user can conveniently search the list for keywords appearing in the subheaders or tool descriptions, or look through the tools in a particular category.

Tier of Tool Information Standard	**# tools**
Sparse	34
Basic details	105
Detailed	589
Highly detailed	5
Comprehensive	21

Table 2. Metadata richness of curated proteomics tools. The number of *bio.tools* entries compliant to different tiers in the Tool Information Standard is shown.

At the outset, EDAM only contained a few terms for proteomics data analysis; many additions and changes were needed, and these were made progressively over multiple EDAM releases. Changes included adding new concepts where these were missing, ensuring the preferred label reflected the vernacular, and adding common synonyms of this term. The conceptual hierarchy (concept subsumption relationships) was also extensively revised, to make navigation of EDAM and term picking easier in ontology browsers. As an illustration, Figure 3 shows spectral analysis operations (EDAM:operation_3214). A particular effort was focussed on the curation of proteomics data formats as these have high practical value in applications such as workflow composition.[10] 30 new mass spectrometry data formats were added, including proprietary formats created by companies to support specific machines and specific commercial software, such as Thermo RAW format (EDAM:format_3712) supported by Xcalibur, and open source data formats such as mzXML (EDAM:format_3654). EDAM overlaps with a few of the concepts within the PSI-MS ontology[11] which is designed to describe a mass spectrometry experiment. Collaborative efforts between the maintainers of both ontologies will be intensified to ensure the interoperability of these ontologies, for example by cross-referencing equivalent concepts.

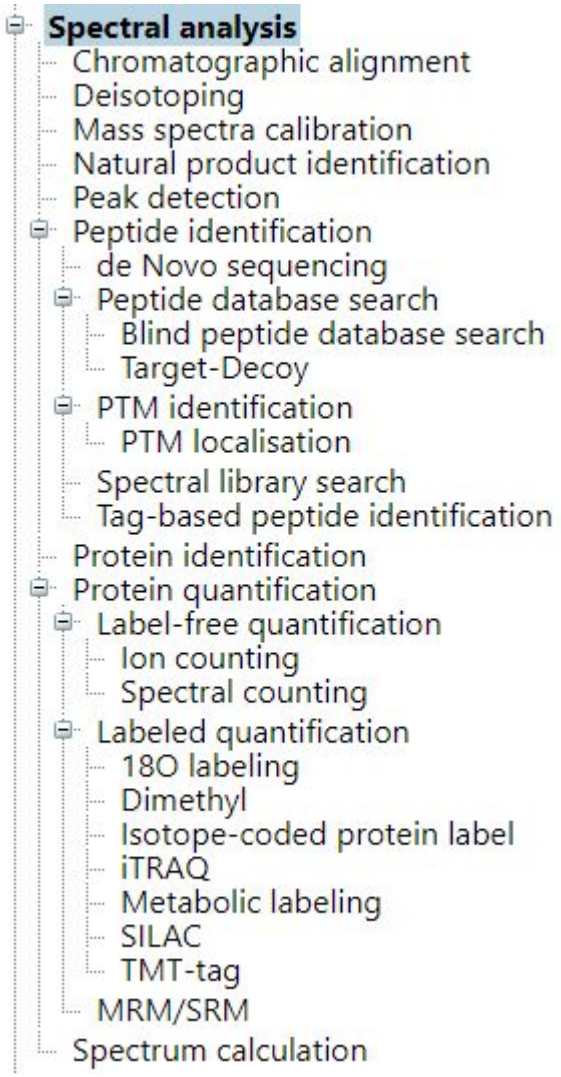

Figure 3. Extract from the EDAM ontology showing operations for spectral analysis (EDAM:operation_3214).

Early community engagement helped to prioritise the curation effort and focus on annotations of high practical value to tool interoperability, such as input and output data formats. The emerging Tool Information Standard was helpful to structure the curation effort on a technical level. It was surprising that in many cases, crucial usage information such as programming language, software license and terms of use, were not easy to find. Basic input and output data types and formats were also often not stated in an explicit and clear manner. As a last resort, supported data formats were identified through inspection of the source code or by testing the tools at the command-line. Such challenges in finding information present a barrier to end-users' efficient discovery and use of tools, and underlines the need for resources such as *bio.tools* and ms-utils.org. To provide consistent search and discovery, these resources benefit greatly from the use of controlled vocabularies defined within biotoolsSchema and the EDAM ontology. The numerous EDAM concepts about proteomics are well described

and documented, and able to represent almost all the functionality found in any proteomics tool, which in combination with ontology browsers such as OLS, BioPortal and EDAM Browser, greatly facilitates the manual annotation of tools.

The proteomics community benefits from consistent and detailed tool annotations in various ways. *bio.tools* allows researchers to query and find appropriate tools with algorithms that fulfill a certain task, with correctly described input and output file compatibilities, and with valuable references to documentation, tutorials and training. Annotations can furthermore be used to compose workflows comprising multiple operations as previously shown[10]. Collections of single tools and workflows executing identical operation(s) for the analysis of proteomics data can be created and benchmarked by comparing the results using ground-truth data sets. We envision that future efforts will result in a feedback loop where valuable information about tool performance will continuously be updated by monitoring their usage and therefore enhance the annotation, presentation and discovery of optimally performing tools.

Conclusion

Organized catalogues of expert-annotated software, like Pedro's list, that describe software using a standardized vocabulary on one platform, facilitate what can be a daunting search for tools that suit a particular scientific or technical purpose. Providing better and more permanent tool findability should automatically lead to longer half-lives, assuming the software to be functional and maintained. We have summarised a successful curation effort that has enriched *bio.tools,* ms-utils.org and the EDAM ontology, and rendered a significant proportion of all proteomics analysis software more findable, accessible, interoperable and reusable, *i.e.* more FAIR.[10,12] While detailed annotation of fine-grained details such as data formats are costly, the effort is warranted where it supports valuable scientific applications such as tool interoperability and workflow composition. Detailed tool annotations including input/output data and format will open the door for identifying novel workflows of compatible tools and for implementing alternative workflow components to benchmark their performance. Such efforts can leverage software containers, for example those being registered in Biocontainers [13] in collaboration with *bio.tools*, with the hope to greatly simplify deployment of full data analysis pipelines on local high-performance machines or on the cloud. BioContainers is providing an infrastructure to create, deploy and maintain software containers using Conda and Docker technologies. bio.tools and BioContainers are coordinated under the ELIXIR Tools Platform (https://elixir-europe.org/platforms/tools). As an example, systematic efforts

are ongoing to ensure that all tools which have been containerised are registered in bio.tools, and conversely, bio.tools is being used to provide metadata for exposure in the BioContainers registry.

The difficulties we encountered in finding sometimes even basic information about tools point to a pressing requirement for the promotion of better standards of information for life science software generally. There is a need for upstream provision of richer and more consistent software metadata that can be conveniently reused by efforts such as *bio.tools*. On the cataloguing side, there is no free lunch; high quality content requires an investment of time and manual effort. The curation effort would benefit greatly from more automated ways to harvest trivial annotations such as software license, for example by text mining the literature, and by a closer integration of the ontology construction and tool registration processes, for example harvesting missing terms and synonyms at tool registration time. The quality of annotations would benefit from more powerful and convenient means for term selection, which itself is a significant challenge given the sizeable vocabularies that the typical end-user, pressed for time, may be unfamiliar with.

We approximate that of the potential volume of 1,097 tools existing for proteomics (see *Sources of information*), *bio.tools* captures 68% (754) with 56% (615) annotated to "Detailed" level or better. Thus, there is more curation work to do, and we can expect many new resources to appear in the future, which will also reflect new analytical methods, types of data and data formats. We recently contacted the developers of tools in the proteomics corpus for which contact details were available in *bio.tools*, and hope this will lead to community adoption and maintenance of the corpus in the long-term. We hope the efforts described here for proteomics will stimulate similar efforts in other domains, which are also witness to a large rise in the volume of new tools and data resources.[14] The anchoring of *bio.tools* within the ELIXIR infrastructure will ensure *bio.tools* is maintained in the long term and we encourage the whole proteomics community to collaborate with us on further improving the corpus of tool descriptions.

Acknowledgements

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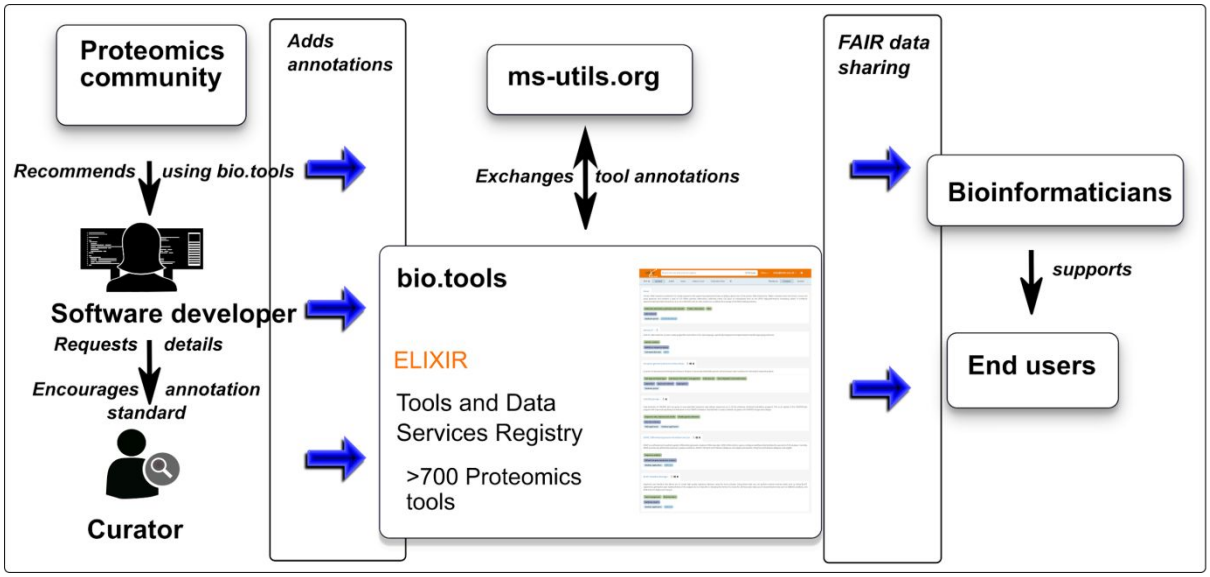
Proteomics community
Recommends
using bio.tools
Software developer
Requests
details
Encourages
annotation standard
Curator
Adds annotations
ms-utils.org
Exchanges
tool annotations
bio.tools
ELIXIR
Tools and Data Services Registry
>700 Proteomics tools
FAIR data sharing
Bioinformaticians
supports
End users

For TOC only