Assessing Value of Biomedical Digital Repositories*

Chun-Nan Hsu[1], Anita Bandrowski[2], Jeffrey S. Grethe[3], Maryann E. Martone[3]

[1]Division of Biomedical Informatics, Department of Medicine, University of California, San Diego, La Jolla, CA, USA.

[2]SciCrunch Inc. San Diego, CA, USA.

[3]Center for Research in Biological Structure, University of California, San Diego, La Jolla, CA, USA.

Corresponding Author:

Chun-Nan Hsu

Email address: chunnan@ucsd.edu

[*] This manuscript was originally prepared as a response to *NOT-OD-16-133 Request for Information (RFI): Metrics to Assess Value of Biomedical Digital Repositories* by the National Institute of Health. C.-N. Hsu presented the contents orally in the 2016 workshop on collaborative data projects, Taipei, Taiwan, December 8, 2016. http://odw.tw/2016/

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Abstract

Digital repositories bring direct impact and influence on the research community and society but measuring their value using formal metrics remains challenging. their value. It is challenging to define a single perfect metric that covers all quality aspects. Here, we distinguish here between impact and influence and discuss measures and mentions as the basis of quality metrics of a digital repository. We argue that these challenges may potentially be overcome through the introduction of standard resource identification and data citation practices. We briefly summarize our research and experience in the Neuroscience Information Framework, the BD2K BioCaddie project on data citation, and the Resource Identification Initiative. Full implementation of these standards will depend on cooperation from all stakeholders --- digital repositories, authors, publishers, and funding agencies, but both resource and data citation have been gaining support with researchers and publishers.

Impact vs. Influence

Assessing the value of digital repositories shares many similar challenges to assessing the value of any scholarly work. One challenge is whether to distinguish between direct impact and broad influence. By direct impact we refer to actual changes that the work brings to the field in terms of outcomes, practices, and methodologies. In biomedical sciences, these include, for example, new drugs or treatments for disease, new models of molecular interactive pathways, new experimental methods, etc. By influence, we refer to how widely the work has been disseminated and viewed across a broad community so that a work can influence other work, either by inspiring new research ideas or preliminary testing of hypotheses. Impact and influence may be correlated but that is not always the case. A highly influential work may have a low direct impact and vice versa. A digital repository may have a high influence in that it is viewed many times, but low impact in that there is no evidence that the actual products are used to advance science. However, the products may be very useful for educational purposes or in planning research. The converse is also true; a digital repository may not be well known across a wide swath of the community, but its products may be highly impactful in a smaller community. Understanding where each resource fits and therefore how to evaluate their success and perhaps

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improve both dimensions requires that it be possible to measure these in some objective and preferably automated or semi-automated way.

Measure vs. Mention

While traditional metrics of a scientific work are based on citations -- whether the work is *mentioned* in scientific publications, digital repositories allow *measures* through the count of access in different ways, URL connections, data transferring, etc. One may argue that measures of access more accurately reflect the value of a digital repository for without access, a digital repository is not used and cannot create value. However, as discussed above, the value of a work may present as impact or influence. Usually, mention-based metrics, such as citations, reflect influence better, for a work can be mentioned only after it is known. However, citations can also reflect actual use of the resource within a published study. Currently, both are hard to track; this makes proper citation of resources and their data products in the literature extremely important.

Measure and mention are not always correlated for a digital repository (Huang et al. 2015; Huang 2016; Rose & Hsu 2016). Moreover, different measure-based metrics, for example, URL connection count, and FTP download count, size of data transferring, are not always correlated. The lack of correlation applies not only when comparing digital repositories but also when comparing content units within a digital repository. Results in (Huang 2016; Rose & Hsu 2016) show that ranking protein structures in RCSB PDB (Protein Data Bank), a data repository of protein structure data, by different measures of access give uncorrelated results. In the study, we ranked protein structures according to their frequencies of Web access (http views) and FTP access (file downloads). We found that *no* protein structures were shared in the top 20 of the two resulting ranked lists. Moreover, the two frequencies are not correlated, in the sense that a protein structure that is highly accessed by Web browsers is not necessarily highly accessed by FTP, and vice versa.

Meanwhile, in addition to citations in publications, mention-based metrics may include citations in press reports, blogs, social media, and other forms of publications, currently measured by services such as Altmetrics (2016). These may not be correlated either, and may better reflect the influence of a work than its impact. Citation analysis is currently hampered by a lack of standard format for such references. Citations may be in different forms, including directly mentioning various names of a digital repository, citing the publications describing a digital repository or mentioning the URL links to a digital repository. For example, an author may cite RCSB PDB by its various publications, URL links to its portal Web page (with different versions throughout the years after it went online), PDB IDs or URL links of protein structures.

Authors not only cite RCSB PDB in different forms, the annual growth rates of the counts of these different citations forms are not correlated for either the data repository as a whole (Huang et al. 2015), or for protein structures (Huang 2016; Rose & Hsu 2016). Authors most frequently chose to cite publications, because usually that is how repositories instruct authors to do in a "how to cite us" page. However, URL link mentions are growing rapidly. Though the PDB ID is designed as a unique ID to mention specifically to a protein structure in PDB, the ID itself is not globally unique without a prefix, and may coincide with a wide variety of entities (Rose & Hsu 2016). PDB IDs are always 4 characters in length. The first character is a numeral in the range 1-9, while the last three characters can be either numerals (in the range 0-9) or letters. Examples of other IDs and/or entities matching this format include "1USD" as currency, "2NO3" as a chemical compound, and "1E10" as a floating-point number; while "1USD", "2NO3" and "1E10" are all legitimate PDB IDs.

(Table 1)

Table 1 shows all the issued PDB IDs presented in full-text format articles. The statistics were obtained from publications containing mentions of PDB ID from the PubMed Central (PMC), where we obtained 1,015,179 articles in NXML format, and 1,093,980 articles in plain text format as of August 2015. Removing duplicate PMC IDs yielded a total of 1,015,233 articles.

(Table 2)

Table 2 compares the top 10 PDB protein structures by the frequency of PDB ID mentions and the top 10 ordered by the frequency that their original publications were cited in the references by subsequent articles in the PubMed. The two lists share only two PDB protein structures (2RH1 and 2A79), suggesting that high PDB ID mentions and high publication citations are not necessarily correlated (Huang 2016). Therefore, relying on either frequency as a sole metric will lead to different assessments of the influence of protein structures.

Standardization of Mentions and Use

Currently, one of the most difficult problems facing assessments of digital repositories is the lack of formal systems of citation that allow measures of influence and direct impact to be calculated using modern information technology. As documented by (Huang et al. 2015), the current means of referencing a digital repository or its content in the literature or any other work involve a range of styles including URLs, reference to a publication describing the resource, accession numbers and free text. Because of this, a very simple question like: how many people have documented use of this resource cannot be answered without resorting to extensive manual labor or advanced natural language processing (NLP) (Rose & Hsu 2016; Ozyurt et al. 2016).

Through the Neuroscience Information Framework, the NIDDK Information Network, the Resource Identification Initiative, and the Data Citation Working groups at FORCE11, we've successfully worked to change this by developing and promoting standards for both resource use and data citation, with a focus on the literature.

Perspectives from the Neuroscience Information Framework. The Neuroscience Information Framework (NIF; Gupta et al. 2008; Gardner et al. 2008) and its sister project, the NIDDK Information Network (dkNET; Whetzel et al., 2015) has been cataloging and tracking the digital research resource landscape for over 8 years. We maintain a large database that tracks how a resource has evolved over the years, including whether it is no longer in service. Currently, a relatively small number of resources (229, List from NIF 2016) are completely out of service; many more, however, grow stale over time. Over time, we have developed some criteria for determining whether a resource is vibrant and growing or moribund: 1) when was the last time a web page was updated on the site; 2) when was the last time data were added; 3) do the data represent a significant fraction of data available in a community or a very limited amount? 4) When a resource is down, does anyone complain? We call the latter the "squawk factor".

As the charge for NIF, established by the NIH Blueprint Consortium, was to determine what resources had been created through NIH-funding and to make them available to the research community, NIF early on worked to develop NLP pipelines to identify resources within the biomedical literature, as most researchers creating resources will publish a paper about a resource like a database or genetically modified organism, or will mention use of specific resources within the materials and methods section of the paper.

The lack of formal or machine-readable standards for referencing these resources within the literature uncovered significant problems in the way that researchers were recording resource usage. These poor reporting standards directly led to the inability of funders or resource providers to track usage or for researchers to identify research resources or find other papers that used them. To address this, NIF worked through FORCE11 to launch the Resource Identification Initiative.

The Resource Identification (#RRID) Initiative (Bandrowski et al. 2016) is designed to help researchers sufficiently cite the key resources used to produce the scientific findings reported in the biomedical literature. A diverse group of collaborators are involved in the project, including the Neuroscience Information Framework which launched and has been leading the initiative, the Oregon Health & Science University Library which contributed significantly to the early pilot project, with the support of the National Institutes of Health and the International Neuroinformatics Coordinating Facility (2016). Resources (e.g. antibodies, model organisms, cell lines and digital tools) reported in the biomedical literature often lack sufficient detail to enable reproducibility or reuse (Vasilevsky et al., 2013). For example, databases are cited by a URL that is no longer available leading to 404 errors, and the version numbers for software programs used for data analysis are often omitted as is the access date of digital repositories.

The Resource Identification Initiative aims to enable resource transparency within the biomedical literature through promoting the use of unique Research Resource Identifiers (RRIDs). In addition to being unique, RRID's meet three key criteria, they are:

1. Machine readable and search friendly.
2. Free to generate and access.
3. Consistent across publishers and journals.

RRID's depend on comprehensive resource registries which provide an authoritative source for each resource type. Each is covered by a different database, e.g., the Antibody Registry, the SciCrunch (NIF) Resource Registry. These databases were aggregated and made available through the Resource Identification Portal (2017), supporting NIH's new guidelines for Rigor and Transparency in biomedical publications. The portal aims to promote research resource identification, discovery, and reuse and offers a central location for obtaining and exploring RRIDs. The current number of digital tools, including databases, software projects as well as commercial tools, listed in the Registry is over 14K (Bandrowski et al. 2016). The number of antibodies is > 2.5M, model animals are in the hundreds of thousands and cell lines over 60K.

The project has been running since 2014. Currently, over 2,500 papers have appeared with RRID's from over 200 biomedical journals. Cell Press has just adopted the standard (Marcus et al, 2016; Cell 2016) and eLife and the Endocrine Society announced that they will be strongly encouraging authors to use RRID's in their journals.

RRID's provide the means for users to unambiguously reference the resources used within a study in their publication. Authors are asked to insert RRID's for resources *used* in their studies after the first reference to the resource in the materials and methods. To ensure that RRID's are easily identified and extractable from the literature, authors are asked to prepend the namespace RRID: before using the database accession number. Thus, RRID's specifically target the use of resource resources as opposed to mentions in an introduction or discussion. A simple search through Google Scholar for an RRID will return papers that have used a resource, e.g., 6 articles have appeared to date that used the PDB (Google Scholar PDB 2016).

RRID's also provide a convenient means for authors to access which digital resources used in papers. Research resource providers can update the registry in the portal when there is a need to transfer the data and software to another repository, but the RRID will remain the same to ensure that readers can always locate the data and software through a centralized registry. This new approach solves data access, sharing, archiving, and preservation at the same time. In addition, it provides a standard citation format that can be easily extracted to show what resources were used in a published study - allowing for measurement of impact. For example, consider FSL, a widely-used software library for functional MRI. Querying Google Scholar with query string "RRID:SCR_002823" will precisely match 26 recent articles reporting research results using FSL. In contrast, querying Google Scholar with keyword "FSL" will overwhelm a user with tens of thousands of hits. In many cases, "FSL" matches an author's initial while others are not related to the software library in question. Since maintaining a correct reference of the RRID increases visibility and thus influence of a research resource, and will bring direct impact eventually, providers of research sources will be highly motivated to maintain its correctness, closing a healthy positive feedback loop to sustain the whole system.

Early adoption of RRIDs already allows us to perform a preliminary study of digital research resources including software, data sets, and Web services in neuroscience. We deployed a software robot called "Scibot" to automatically annotate RRID mentions in research articles on the Hypothes.is (2017) Web annotation platform. A team of curators of SciCrunch then continued to manually curate each automatically annotated RRID mentions with Hypothes.is. In this way, we could rapidly collect RRID mentions. By August 1, 2016, we have collected 2493 curated mentions from 757 articles. Figure 1 shows a histogram of the number of unique RRID mentions identified in an article. The histogram shows that most of articles contain more than one unique RRID mentions, providing an opportunity to analyze correlation between research resources based on their co-mention partners in publications.

(Figure 1)

Table 3 shows the top 30 highly mentioned RRIDs from this data set. Though the data set is biased toward early adopters of RRIDs, the list shows an interesting mix of general-purpose image analysis/statistical tools and neuroscience specialized resources that are widely used by the neuroscience research community. We have also developed fully automatic text mining methods (Ozyurt et al. 2016) to complement the curation approach to perform comprehensive analysis of the impact and influence of research resources in life sciences.

(Table 3)

Data Citation Implementation Pilot Project (2017). RRID's address the citation of digital repositories and associated tools at a high level; however, we also need a system to cite individual data sets that may include only a subset of data in a repository or be assembled from multiple data sources. Precisely referring to which subset of data is retrieved and used can be a computationally intractable problem, which leads to some pessimistic views regarding data citation (Buneman et al. 2016).

We argue that the ultimate purpose of data citation is not only to identify precisely a data subset for facilitating reproducibility, but also to ensure that both the individuals contributing data and the repositories housing them receive proper credit and attribution, as specified in the Joint Declaration of Data Citation Principles (JDDCP, Data citation 2014). The JDDCP has been endorsed by 253 individual scientists and 114 organizations, representing different sectors of stakeholders, including data centers/data repositories, educational institutions, funding agencies/organizations, libraries, publishers, registries/social networks/research networks, societies/associations/consortiums, and technology providers.

Based on the eight principles given in JDDCP, FORCE 11 and other groups have been working on developing practical standards to implement data citations. One of these is the Data Citation Implementation Pilot Project (DCIP) as part of the NIH BD2K bioCADDIE (2017) project that we have been working on. The primary goal is to provide basic coordination between publishers, repositories and identifier / metadata services for early adopters of data citation according to the JDDCP. To meet this goal, we will provide authoritative guidance and group consultation on data citation implementation to help establish one or more benchmark implementations of data citation based on the JDDCP and Starr et al (2015), its cross-domain implementation guidance.

The key ideas here include working with data repositories on best practices that repositories can follow to support data citation with the support of community metadata standards, the use of persistent identifiers (e.g., DOI's), and machine-readable landing pages, which provide essential information on the content and accessibility of data within the data repository (Cousijn et al. 2017; Fenner et al. 2016). A landing page allows for an access point that is independent from any multiple encodings of the data that may be available (Starr et al. 2015), and thus avoids the complicated computational problem of citing arbitrary subsets of data precisely, as described in (Buneman 2016). A landing page can also provide information on access controls required by licensing or privacy considerations. In addition, user requested landing pages can be minted for custom data aggregations as well.

We are often asked how RRID's differ from the referencing of a specific data sets as proposed by the JDDCP. The issue is one of granularity. RRID's are meant to identify the parent entity like the PDB, while additional identifiers may be used to identify the specific data set used. This more granular data citation may comprise a subset of a data repository or a supra-set across repositories. The RRID essentially functions as an ORCID to identify the organizational entities involved, e.g., the data repository, while the DOI points to a specific and unique data set. DataCite (2017) and Dryad (2017) are closely related to RRID. They assign persistent identifiers (e.g., DOIs) for research data, especially data sets that do not fit well into thematic data repositories that contain data sets organized to serve the research needs on common topics such as PDB. They also provide permanent storage space for these data sets. DataCite and Dryad complement the efforts of RRID, which covers a broader range of research resources including thematic data repositories. GRID (2017) releases the IDs and metadata for research organizations and data providers to use under the Creative Commons Public Domain 1.0 International licence. GRID maintains well curated hierarchies of research organizations (e.g., a lab within a department in a university) and is useful for accurate identification of research resources with its uniquely distinguishable IDs of provider organizations.

Towards Reliable and Accurate Metrics

Though counting frequencies of standardized RRID mentions and data citations might not be the single perfect metric of the value of a digital repository, widespread adoption of these standards will lead to a more reliable and comparable metric than the status quo and open development of more sophisticated metrics like the h-index (Hirsch 2005) and pagerank (Page 1999) derived from raw frequencies of literature citations. However, unlike publications, authors may cease to credit and mention highly used resources that become routine, such as PubMed. This is when access statistics may provide a better metric to assess their value. Also, accurate mention identification measures influence at best. Assessing impact will requires not only provenance of research outcomes to their various digital and data repositories contributing to their development but also the impact of the research outcome in question, for which a general acceptable metric is not currently available, and usually the impact may take years or decades to reveal.

A potential remedy for these issues is to request authors to explicitly distinguish why they chose to mention a digital repository -- whether they used the data or service to obtain their results, or they are merely related. Even without explicit citation mechanisms, it may be possible to make the distinction to some extent from the context where the mentions appear (e.g. in the methods section it may suggest that the data was used), and therefore distinguishing whether the data or service lead to direct impact (a mention indicates influence of the resource in some way already). Similarly, it would be possible to distinguish whether the mention carries positive or negative sentiment of the resource. The key is that the standards bring unambiguous and persistent references to digital repositories.

Funding Statement

The research reported here is supported in part by Grant U24AI117966 National Institutes of Health Big Data to Knowledge (BD2K) Initiative, U24DK097771 National Institute of Diabetes and Digestive and Kidney Diseases, and U24DA039832 National Institute on Drug Abuse.

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Tables.

Table 1. Different types of mentions of issued PDB IDs identified in PMC. The statistics of mentions may include false positives due to errors by the text mining software for the last two types.

Identifier	Example	Machine readable	Mentions(*)	%
PDB ID	PDB ID: **1STP**	yes	14,888	4.8
PDB DOI	http://dx.doi.org/10.2210/pdb**1stp**/pdb	yes	155	0.05
External link tag	<ext-link … ext-link-type=”pdb” xlink:href=”**1STP**”>	yes	32,108	10
PDB file name	**1stp**.pdb	yes	895	0.03
PDB URL	http://www.rcsb.org/… /structureId=**1stp**	yes, but URL may change	657	0.2
Non-standard PDB ID	PDB code: **1STP**, PDB reference **1STP**, PDB accession number **1STP**, Many variations...	yes/no	22,081	7.1
PDB in context	“We employed the following **PDB** coordinates: glycogen phosphorylase, **1gpy** …”	yes/no with text mining	16,726	5.4
Free text	“We first placed S2 bound to human PI3KC; (**3ene**) into the reference coordinates …”	yes/no with text mining	221,287	72

Table 2: Top 10 highly cited protein structures (top) and top 10 highly mentioned protein structures in PDB. “Year” shows when the PDB ID was issued.

Citation Rank	PDB ID	Year	# of Citations	# of Mentions	Mention Rank
1	1AOI	1997	1527	31	37
2	1BL8	1998	1234	35	24
3	1F88	2000	957	44	16
4	1GC1	1998	852	26	57
5	1RV1	2004	747	11	488
6	1FFK	2000	746	31	34
7	**2RH1**	2007	682	124	1
8	1YSG	2005	650	6	1984
9	**2A79**	2005	635	49	10
10	1AIK	1997	561	12	403
Mention Rank	PDB ID	Year	# of Mentions	# of Citations	Citation Rank
1	**2RH1**	2007	124	682	7
2	1UBQ	1987	96	222	142
3	1KX5	2002	69	272	87
4	2R9R	2007	65	433	20
5	3EML	2008	65	408	24
6	1U19	2004	64	227	134
7	1K4C	2001	59	454	18
8	2VT4	2008	55	356	38
9	2B4C	2005	55	289	71
10	**2A79**	2005	49	635	9

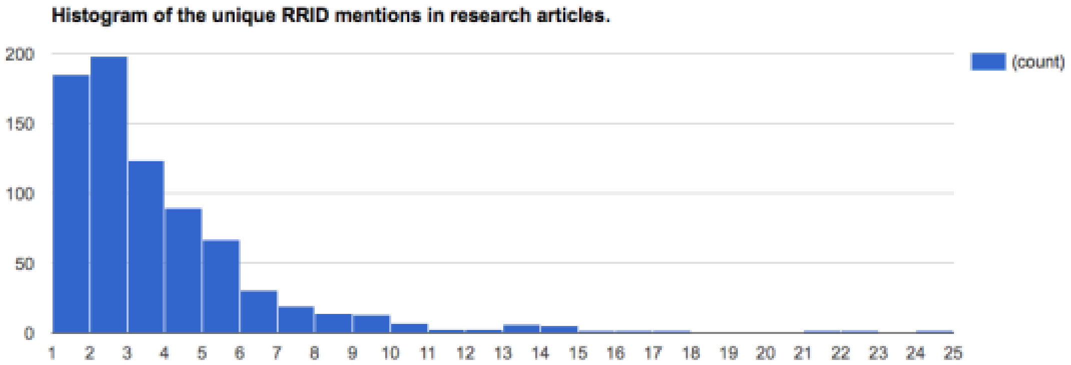
Table 3. Top 30 highly mentioned resources in neuroscience RRID early adopters.

RRID	count	resource name
SCR_003070	260	imageJ
SCR_002798	156	Graphpad Prism
SCR_014199	138	Adobe Photoshop CS5 CS6
SCR_001622	106	MATLAB
SCR_002865	64	SPSS
SCR_001775	57	Neurolucida
SCR_001905	50	R software
SCR_011323	46	pClamp
SCR_002677	35	AxioVision
SCR_007037	34	SPM
SCR_013672	32	Zeiss Zen software
SCR_002078	31	Adobe Photoshop CS2
SCR_002285	29	Fiji
SCR_014198	28	Adobe illustrator
SCR_013726	23	G*Power software
SCR_003238	22	Open Science Framework
SCR_002823	21	FSL
SCR_002526	20	Stereo Investigator
SCR_008520	20	FlowJo
SCR_001847	19	FreeSurfer
SCR_000903	18	Spike 2 software

SCR_007369	17	Image-Pro Plus
SCR_002368	17	MetaMorph Microscopy Automation and Image Analysis Software
SCR_000325	16	IGOR Pro
SCR_003210	16	Sigma Plot
SCR_007353	15	Advanced 3D Visualization and Volume Modeling
SCR_013673	15	Leica AS AF software
SCR_001818	12	NeuroExplorer
SCR_008567	11	Statistical Analysis System
SCR_002716	11	Synapse Web Reconstruct

Figures.

Figure 1. 573 out of 757 articles contain more than one unique RRID mentions. One of them contains as many as 24 unique RRID mentions.


Histogram of the unique RRID mentions in research articles.
(count)