Open laboratory notebooks: good for science, good for society, good for scientists [version 1; referees: 1 approved with reservations]

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Abstract
The fundamental goal of the growing open science movement is to increase the efficiency of the global scientific community and accelerate progress and discoveries for the common good. Central to this principle is the rapid disclosure of research outputs in open-access peer-reviewed journals and on pre-print servers. The next bold step in this direction is open laboratory notebooks, where research scientists share their research — including detailed protocols, negative and positive results — online and in near-real-time to synergize with their peers. Here, we highlight the benefits of open lab notebooks to science, society and scientists, and discuss the challenges that this nascent movement is facing. We also present the implementation and progress of our own initiative at openlabnotebooks.org, with more than 20 active contributors after one year of operation.

Keywords
open lab notebooks, open science, peer-review, preprints, publishing, science communication

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Introduction

The function of the scientific peer-reviewed system is to provide greater confidence that published research is scientifically sound. This system is widely accepted as the best available, although imperfect (as peer reviewers may miss technical flaws or be biased)\(^1\), to guide the global scientific community towards progress. Peer-reviewed publishing is also used by research scientists, funders and institutions as a mechanism to claim ownership of their discoveries. As a result, the community widely believes that findings should be kept secret until they are published in a peer-reviewed journal. This tradition of secrecy, which protects the scientist as opposed to the science, has been transmitted from mentor to trainee for centuries (Galileo kept his discoveries to himself until they were published). In the life sciences, this belief can reach near-mystical levels\(^2\). The peer-review and publication process grew in an era where communication was largely in paper format. Today, in the age of instant communication, one would imagine there should be more efficient ways to operate.

Open lab notebooks: good for science and society

We believe that open laboratory notebooks, where research scientists record their work online and in near-real time, are an efficient way to disseminate data before it is published in peer-reviewed journals, and has several advantages over the traditional “release after publication” system. First, making the data accessible within weeks rather than keeping it hidden for years means that others will be able to build upon the research, and avoid spending time and resources on redundant experiments\(^3\). Second, open lab notebooks should include detailed protocols that can be reproduced, which is often not the case in peer-reviewed publications\(^3,4\). Third, negative data, which are almost never disclosed in the current publishing system but are provided in open lab notebooks, can sometime provide important insight\(^5\). Fourth, open lab notebooks offer a space for anyone to comment on experimental records. This allows experts to provide insight, but also to flag technically unsound experiments, thereby reducing the potential for flawed science to appear in peer-reviewed journals and in pre-print media. Open lab notebooks can therefore help save time, resources, and knowledge. If adopted by many, they should lead to a more synergistic way to do science and to more efficient use of public funds.

Good for scientists

Many believe that openly sharing work online will limit career opportunities. We argue that open lab notebooks have compensating advantages that are good for scientists. To succeed in academia, one must get funding, assert primacy over discoveries, be known in a field of research and be able to present work and ideas clearly and convincingly. Open lab notebooks can help in all aspects.

First, funding agencies are seeing the open science movement as a long lasting and far-reaching shift for the best, and are increasingly supportive of efforts to embrace open science principles. For instance, the symposium set to launch openlabnotebooks.org was entirely sponsored by the Wellcome Trust and the Canadian Institute of Health Research, and senior representatives from the Gates Foundation and the Chan-Zuckerberg Initiative were also in attendance (https://www.thescg.org/open-lab-notebooks-2018). The NIH’s National Institute on Aging dedicated an entire session to open science at their 2018 Alzheimer’s research summit (https://www.nia.nih.gov/research/nih-ad-summit-2018-program-agenda), as did the 2018 Enroll-HD congress of the CHDI Huntington’s Disease Foundation (https://www.enroll-hd.org/enroll-hd-congress-2018/). The Wellcome Trust has recently launched the Wellcome Open Research publishing platform and Open Research Fund. Grant applications that highlight the use of open lab notebooks are being viewed positively. For example, Huntington’s disease (HD) research funders such as the CHDI Foundation, the Huntington Society of Canada and the Huntington Society of America, have all generously funded studies of HD biochemistry at the SGC Toronto.

Second, results in open lab notebook are date-stamped, thus claiming temporal priority of the data. Indeed, public repositories such as Zenodo\(^6\) add a date-stamp to depositions, and assign a citable DOI to open lab notebook records (detailed below).

Third, early career scientists can use their open notebooks to connect with their peers and with experts in the field, start new collaborations and build their own network. Fourth, the use of open lab notebooks provides opportunity to present work clearly and concisely to both experts and non-experts. This is an important skill to master in order to write convincing grant applications. Fifth, junior scientists will also find their open lab notebook a good medium to showcase their technical skills and scientific insight, and may find it useful to add a link in their resume when applying for their next position. Finally, many will find a personal satisfaction in embracing open science and FAIR data principles\(^7\).

Implementation of an open lab notebook platform

Following our prediction that open lab notebooks should be good for science and good for scientists, and after a 2-year pilot study where Rachel Harding, a post-doctoral fellow at the Structural Genomics Consortium (SGC) shared her work on Huntington’s disease at labscribbles.com (https://www.vox.com/2016/3/3/11148452/science-blog), we launched openlabnotebooks.org in January 2018, where 12 scientists from the SGC started reporting their work live, online\(^8,12\). Each post is composed of two documents. (1) A detailed and rigorous experimental record, including all data and protocols, which experts can evaluate, comment on or build upon (Figure 1); (2) a blog, aimed at the non-specialist that explains in simple terms the motivation and rational for the experiment, summarizes results – positive and negative – and outlines next steps (Figure 2). The blogs, posted at openlabnotebooks.org, are managed by a webserver downloaded from wordpress.org and link to the experimental records, which are deposited at Zenodo (zenodo.org), but can also be made available from other public repositories, such as GitHub (github.com) or Figshare (figshare.com). The Zenodo repository enables sharing research outputs from across all fields of research, creation and curation of complete digital repositories, flexible licensing with controlled degree of openness and safe storage of the data for the future in the same cloud infrastructure.
Viability screen of ACVR1/ALK2 inhibitory compounds on Diffuse Intrinsc Pontine Glioma cells

Brown, Elizabeth; Farnie, Gillian; Bullock, Alex

Six compounds developed by M4K Pharma to inhibit the ACVR1/ALK2 tyrosine kinase where tested for their ability to reduce viability of both mutant and wild-type ACVR1 DIPS cell lines (HSU-D-DIPS-007 and HSU-D-DIPS-011 respectively). Compounds where tested on cells grown as 2D sheets and 3D neurospheres as well as with and without radiation treatment. M4K209 was highly effective in ACVR1 mutant DIPS cells, but this was not the case in ACVR1 wild-type cells.

Figure 1. Detailed experimental records including protocols, positive and negative data are posted on Zenodo. A citable DOI is automatically generated (right-middle panel), and the number of visits and downloads provided (top right).

as CERN’s own LHC research data. While the experimental details posted at Zenodo are important scientifically, the blog written in layman’s term can be used to engage with scientists that may have a complementary set of expertise for future collaborations as well as other stakeholders in the research process, including patient groups, a dimension that most in academia are missing.

The ultimate goal of this open lab notebook initiative is not only to increase the impact of our work but also, along with precursors in the field such as Open Source Malaria (http://opensourcemalaria.org/) and other isolated open lab notebook efforts, to inspire others to follow, and contribute to the creation of a new open science movement in the life sciences. While it is too early to judge the success of this initiative, the number of contributing scientists and institutions is steadily increasing (Figure 3). While only one scientist was contributing in November 2017, 23 scientists from six institutions (University of Toronto, University of Oxford, University of North Carolina, University of Leicester, the Karolinska Institute in Sweden and University of Montpellier in France) are recording their work at openlabnotebooks.org as of December 2018.
Figure 2. A blog explains in language accessible to non-scientists (such as patient groups) the rationale and take-home message of the experiment.

As importantly, impact is also increasing, judging by the average number of views per experimental record calculated from statistical data available at Zenodo.org (Figure 3). Some reports raised a considerable interest. For instance, the crystal structure of USP5 in complex with small molecule fragments has 821 unique views and 324 unique downloads as of December 2018. If the initiative is successful, we anticipate that within three to five years, usage metrics are comparable at openlabnotebooks.org and bioRxiv, the preprint server for biology.

Data posted at openlabnotebooks.org is of direct relevance to patient groups. For instance, four scientists record their results on testing chemical inhibitors of the kinase ALK2, a potential therapeutic target for the treatment of the pediatric brain tumor diffuse intrinsic pontine glioma (DIPG), and the heterotopic ossification disorder fibrodysplasia ossificans progressive (FOP). The compounds, developed by the open science biotech company M4KPharma, are still in pre-clinical phase of development but should ultimately lead to clinical trials for these incurable diseases. Scientists working on projects with a clear path to the clinic are eager to share their enthusiasm and commitment with patient groups (sometimes using social media to announce their latest open notebook post) who, in turn, follow their work.

The challenges of open lab notebooks

Three antagonizing points that inhibit scientists from starting their own open lab notebook are the fear of being scooped, the inability to report collaborative work when collaborators want to do so, and the absence of a clear path to the clinic for their research. To overcome these challenges, it is important to provide clear guidelines for data sharing, to encourage collaboration among scientists, and to ensure that the research reported is of direct relevance to patient groups.
to keep data secret, and the concern that an open notebook will take time away from an already overburdened schedule\textsuperscript{17}. The language barrier for non-native English speakers, and the availability of open lab notebook solutions can also be challenging. It is indeed likely that maintaining an open lab notebook increases the chances of being scooped, but it is too early at this point to know whether this effect is minor or significant. Paradoxically, and given the territorial nature of the current frameworks for funding and managing scientific research, entries in one’s open lab notebook may mark one’s area very effectively, especially in a conceivable future when funding trusts and councils start looking into them. We would argue that most, if not all, scientists get scooped during their career, and that open lab notebooks serve as a safety net for early career scientists who have a citable record of their work if they ever get scooped. Obtaining permission from collaborators to report collaborative work in open lab notebooks can be challenging. We believe that the best way to avoid such a situation is to clearly state at the outset of a collaboration the intention to adopt open science principles\textsuperscript{18}. Scientists are more likely to agree if presented with the idea well in advance. The time invested in practicing clear, concise and engaging scientific writing is not lost on one’s career. After some practice, maintaining an open lab notebook should not take more time than using a regular lab notebook.

Future directions and conclusion

Open lab notebooks represent a major departure from current practices in science (especially biomedical sciences) and hold a mix of promises and risks. As the community producing these lab notebooks is increasing, there is an opportunity to move beyond ideology and anecdotal data to evidence-based policy design. In the spirit of openness, we call on colleagues from both the life science and the social sciences communities to conduct systematic evaluation of the benefits and downsides of open lab notebooks. It will be important to compare several parameters on a yearly basis. These may include the frequency of research being scooped among scientists disclosing their work in open lab notebooks versus a less open reference group; the frequency of new collaborations; the frequency of comments and ideas received by the authors of open notebooks; and instances where open lab notebooks were essential for compliance with funder or institutional requirements. More difficult to assess will be issues such as recognition, career progression, speeding up research, and impact on reproducibility, but they could all be addressed with appropriate questionnaires and data analytics.

Our goal is to see the number of open lab notebooks increase exponentially over the coming years. Future implementation of novel features, such as the ability to search for experiments containing compounds with specific chemical templates, is expected to extend the reach of the platform to medicinal and computational chemists. Indexing of open lab notebooks by popular search engines such as Google Scholar (which already indexes pre-prints and other non-peer-reviewed documents) would increase the visibility and impact of open notebooks. Importantly, open lab notebook data deposited at Zenodo.org is already searchable with Google’s Dataset search engine. To further encourage scientists to break free from the tradition of secrecy that has been passed on for generations, a cultural change needs to be supported at institutional and governmental levels. Funding bodies are starting to define and enforce open science publication practices\textsuperscript{19}. Similarly, universities could take a more proactive role, for instance by including adhesion to open-access principles as an evaluation criteria for career advancement\textsuperscript{20}. Indeed, while strong incentives described above already exist for junior scientists to start their own open lab notebook, the benefit to their PIs who already have established a professional network and don’t need to showcase their skills is not always as clear. As long as scientists are not convinced that open science is good for them, Science 2.0 will have to wait.

Data availability

No data are associated with this article

Grant information

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References

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This opinion piece is on a timely, important topic and is clearly and engagingly written. Anecdotally, we find that many of our colleagues in science are unaware that open lab notebooks exist. This article will help.

The authors identify several important advantages and challenges associated with the near-immediate deposition of results into the public domain, online. They use examples from their own research to highlight the possibilities.

The refereeing team behind this review are seasoned users of open lab notebooks, and so are in a good position to judge the piece. We judge it to have cleared peer review from our perspective, once the following comments and suggestions have been acted upon. There are a number, which should be read not as criticism but as testament to our shared enthusiasm for this subject and its importance in the future of research.

1) Secrecy. In the introduction, reasons are suggested for why scientists may keep results secret. We would suggest that there are two important reasons that are not explicitly mentioned: i) that the scientist may want to patent something, and ii) that the scientist cannot be bothered to work out how to release research using atypical means. The first point is alluded to where mention is made of ownership, and the second point is alluded to by the mention of "paper" but we would argue these two factors are significant enough that they should be made explicit.

2) Careers. We'd be interested in whether there is a justification for the statement "Many believe that openly sharing work online will limit career opportunities." If there is none, then perhaps rephrase this more as a possibility?

3) Grants. The statement "Grant applications that highlight the use of open lab notebooks are being viewed positively" may be true (one hopes it is), but the evidence presented doesn't support that statement (the grants may have been funded because the science was so good, regardless of the dissemination plan), so again, this probably needs to be made more aspirational.

4) Errors. The authors need to address what happens if an experiment is recorded containing a mistake, and a mistake that might propagate via an ungrounded conclusion. Is there a danger in leading
colleagues down the wrong path? Is there a danger to the reputation of young scientists? Would incorrect conclusions, if indexed by search engines, lead to literature pollution that might be hard to correct?

5) **Machines.** One must make the assumption that few people will ever read open lab notebooks, just as few people read regular lab notebooks. More needs to be made of this, since a) it is essential, rather than just desirable, that the notebook is searched and indexed by e.g. Google, and b) the entries need, ideally, to be machine readable. Could the authors comment on this - i.e. how Googletable the contents are (beyond the Dataset Search they mention) and what can be done to ensure that the entries can be understood by machines?

6) **Permanence.** There are many web links in the article. This is an academic publication, which is intended to last forever. It's likely those URLs will not last forever. Is there a way that the pages pointed to can be archived somehow? An important, relevant example: this manuscript does not refer to one of the pioneers of open lab notebooks - indeed he coined the phrase "open notebook science" - Jean-Claude Bradley. Bradley's blog can still be accessed but the wiki that used to house all the raw data has gone. In publishing our most recent paper that made use of open lab notebooks¹, we took pains to archive the lab notebooks on a repository to mitigate potential loss by external providers, and to back up web pages (as PDFs) to similar places. Can the authors address the two issues here: i) should we link to web pages in academic articles without backing them up? 2) How are the lab notebooks backed up and archived?

7) **Time Stamps.** The authors mention "results in open lab notebook are date-stamped." It would be interesting to know whether the authors have looked into whether the date stamps are "convincing" from a legal standpoint. Would they, for example be sufficient to claim priority in a legal challenge? Is there an issue with the fact that ELN pages can be edited, over an extended period of time, or is it sufficient to ensure that the page has a robust revision history?

8) **Scooping.** A scooper could claim that they were simply unaware of the open scientist's work. This seems a reasonable defense. What needs to happen for ignorance of an open lab notebook not to be a defense against ignorance of prior art?

9) **Citations.** We are cited twice (thank you), but there are two other relevant papers the authors might be interested in citing should these be deemed by them to be appropriate: i) an extensive discussion on the use cases of an open source ELN called Labtrove² pioneered by Jeremy Frey's team at Southampton, and ii) a large medchem project by Open Source Malaria which was conducted entirely using open lab notebooks ¹ and which may be instructive in terms of how to publish a paper based on open notebook work (also described informally here.

10) **Examples of Inputs.** Are there any examples the authors can point to where the open ELN has helped the research, e.g. where suggestions have been made, and acted upon, to help the science?

11) **Examples of ELNs.** Are there other examples of open lab notebooks being used in biomedical research? Is this, in fact, still a highly niche activity?

12) **Language.** The language barrier is mentioned, but we're not sure this is relevant to this paper. Language is already a barrier in the current system, though English is essentially a *lingua franca* across science.

13) **Licence.** What is the license that covers the authors' i) blog posts and ii) notebooks? To what extent is this an important choice? For example, can others take and re-use the content without restriction, or
only for non-commercial purposes?

14) **Raw Data.** The authors mention that the ELN entries include "all data". This is an important feature of open ELNs that distinguishes the practice from a great deal of open science in which highlights might be discussed, or blogged about, but without the attendant raw data. We investigated briefly to see how much of the raw data could be accessed in the authors' cases. We have noticed that a fair number of the lab notebook entries recorded by the team in Zenodo contains PDF/Word-style summaries of data, rather than the data themselves. This limits re-use of the data. Could the authors comment on the central importance of the availability of all raw data?

Examples:
- This blog post mentions performing synthesis of analogues based on lit procedures but there’s no link to an ELN.
- Same with this page.
- And this.
- This page has a link (in the 2nd paragraph) to a (structure?) data file but no backlink from the data back to the blog page, risking orphaning of content?
- This blog page does have a link to the ELN. There is more experimental detail, but there is no raw characterization data. Also the backlink to the blog page is broken.
- Many biology entries contain pictures of purifications and for the most part, the ELN pages only have a docx or pdf there. Should there be any raw data available for these kinds of pages, or are docx and PDF enough?

15) **Identifiers.** It is mentioned that is is desirable to have "the ability to search for experiments containing compounds with specific chemical templates". We agree. Some ELNs already allow this (e.g. Chemotion and C6H6 4). We have found a stop-gap is the manual inclusion of chemical strings such as SMILES, InChI. Can the authors comment on whether similar things can be included in order to allow machines to understand the biology contained within the entries, e.g. UniProt numbers?

16) **Metrics re Access.** Is there a way of distilling out access by non-team people, or even access by the author of the page who may have accessed multiple times during the editing of a page?

17) **Ownership.** When a researcher moves on, does that researcher have any responsibility towards the ELN? e.g. if a mistake is found, who needs to correct it? Is it the responsibility of the PI to act as future curator?

**References**
researcher-centric ELN. *Chem Sci.* 2015; 6 (3): 1614-1629


Is the topic of the opinion article discussed accurately in the context of the current literature?
Partly

Are all factual statements correct and adequately supported by citations?
Partly

Are arguments sufficiently supported by evidence from the published literature?
Partly

Are the conclusions drawn balanced and justified on the basis of the presented arguments?
Partly

**Competing Interests:** No competing interests were disclosed.

**Referee Expertise:** Open source drug discovery, organic and medicinal chemistry

We have read this submission. We believe that we have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however we have significant reservations, as outlined above.

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