# Opening doors to physical sample tracking and attribution in Earth and environmental sciences

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# Abstract

Physical samples and their associated (meta)data underpin scientific discoveries across disciplines and can enable new science when appropriately archived. However, there are significant gaps in current practices and infrastructure that prevent accurate provenance tracking, reproducibility, and attribution. For most samples, descriptive metadata are often sparse, inaccessible, or absent. Samples and associated (meta)data may also be scattered across numerous physical collections, data repositories, laboratories, data files, and papers with no clear linkage or provenance tracking as new information is generated over time. The Earth Science Information Partners (ESIP) Physical Samples Curation Cluster has therefore developed guidance for scientific authors on 'Publishing Open Research Using Physical Samples.' This involved synthesizing existing practices, community feedback, and assessing real-world examples. We identified improvements needed to enable authors to efficiently cite and link Earth science samples and related data, and track their use. Our goal is to help improve discoverability, interoperability, and reuse of physical samples, and associated (meta). Though primarily focused on the needs of Earth and environmental sciences, these guidelines are broadly applicable.

# Introduction

Physical samples and their associated (meta)data are primary building blocks across a wide range of scientific research. They represent features of interest or living things<sup>1,2</sup>, underpin discoveries across disciplines, and are critical to the scientific process. For example, these may include soil or water samples collected to represent environmental conditions, a rock from a geologic outcrop, or a preserved organism. When samples and associated (meta)data are findable, accessible, interoperable, and reusable (FAIR)<sup>3</sup> and as "open as possible"<sup>4–6</sup>, new science becomes possible<sup>7,8</sup>. For example, users can instantly integrate and download species occurrence records published in <u>Global Biodiversity Information Facility (GBIF)</u> from over 2,000 institutions/sources globally. As a result, GBIF records are used frequently in new synthesis studies and are cited in more than two publications per day<sup>9</sup>. However, for many data types and disciplines – including Earth and environmental sciences – widespread adoption of standard practices and tools for sample and (meta)data discovery, integration, and use are in more immature stages<sup>10</sup> or do not yet exist. This paper seeks to outline practices that enhance sample and (meta)data discovery in Earth and environmental sciences, and increase the pace of new scientific insights.

Progress in funding policies, standards, and infrastructure for samples continues to motivate greater discovery, sharing and reuse of samples and associated (meta)data<sup>9,10</sup>. Recent updates to the U.S. National Science Foundation (NSF), Division of Earth Sciences (EAR) Data and Sample Policy require that:

*"All data and sample metadata underlying peer-reviewed scholarly publications resulting from EAR support must now be made publicly accessible at or before the time of* 

publication, and no later than two (2) years after completion of data collection or generation, via appropriate long-lived FAIR-aligned repositories<sup>711</sup>.

However, there are significant infrastructural and sociotechnical gaps that prevent accurate provenance tracking<sup>12</sup>, reproducibility<sup>7,13</sup>, and attribution<sup>14,15</sup>. For the vast majority of samples, descriptive metadata are often sparse, inaccessible, or absent<sup>16–18</sup>. Samples and associated (meta)data may also be scattered across numerous physical collections, data repositories, laboratories, data files, and papers with no clear linkage or provenance tracking as new information is generated over time<sup>12,19</sup>. Yet, there is a growing need to connect related interdisciplinary sample-associated (meta)data spanning diverse fields and data systems<sup>20</sup>.

There is also a need for researchers to respect Indigenous Data Sovereignty and Governance for samples collected on lands and waters belonging to Indigenous Peoples and track appropriate use of such samples. While beyond the scope of the current work, researchers should be aware of and uphold the CARE (Collective Benefit, Authority to Control, Responsibility, and Ethics) Principles for Indigenous Data Governance<sup>21</sup> for both the collection and long-term management of samples and any derivative data on those samples.

Overall, practices for publishing and citing sample-associated data have been inconsistent, and there is a lack of clear guidelines across disciplines. This has led to several consequences: 1) Research that uses samples may not be reproducible<sup>7</sup>; 2) It can be time-consuming or even impossible to track related data and information about samples<sup>22</sup>; 3) Samples can be difficult to find and reuse; 4) Sample collection managers are less able to show the impact of their collections and curatorial work<sup>15</sup>.

To address these challenges, as part of the Earth Science Information Partners (ESIP) <u>Physical</u> <u>Samples Curation Cluster</u>, we sought to develop recommended practices for publishing and citing physical samples in scientific research. The focus here was on field-collected physical samples in Earth and environmental sciences, and associated subsamples and/or derivative data that may span the Earth, environmental and biological disciplines (e.g., microbial genomics subsamples and data from a parent soil sample, associated plant data). We first briefly review existing community practices and infrastructure to enable sample publication, citation, discovery and tracking. We present four use cases that exemplify how sample metadata sharing, citation, and tracking need to be improved. These cases respectively demonstrate efforts to:

- 1. Efficiently publish and cite large numbers of samples and associated (meta)data;
- 2. Provide attribution and credit for those involved in physical sample collection and curation to demonstrate the value of investing in collections;
- 3. Track the use of sample data generated by analysts and laboratories; and
- 4. Connect related interdisciplinary sample (meta)data and other research outputs.

We then outline recommended practices for Earth and environmental scientists publishing sample-related work, which are meant to support these use cases. Finally, we discuss planned future work, existing obstacles, and proposed solutions to improve (meta)data discovery, integration, and attribution for physical samples.

### **Existing Community Practices and Infrastructure**

To develop consistent guidelines for researchers using samples and associated (meta)data in publications, we first surveyed existing community practices and infrastructure regarding 1) standard sample metadata; 2) sample identification; 3) publishing samples and associated (meta)data; and 4) sample citation. Example organizations that provide infrastructure, recommendations, or policies for managing samples and associated data are provided in <u>Supplemental Table 1</u>, with additional information summarized in this section.

#### Standard Sample Metadata

Formal standards organizations have developed, and continue to maintain and expand, metadata standards for describing physical samples in specific disciplines, such as the Open Geospatial Consortium (OGC)<sup>23</sup>, Genomic Standards Consortium (GSC)<sup>24</sup>, and Biodiversity Information Standards (TDWG)<sup>25</sup>. Ad hoc groups have also come together to define metadata formats and templates for specific communities<sup>26</sup>. While beyond the scope of the present work, a previous review compared these existing metadata templates and standards to describe physical samples<sup>27</sup>, which are available for biodiversity records<sup>25</sup>, omics material<sup>28</sup> (such as genomics, metagenomics, metabolomics), earth and environmental science samples<sup>29,30</sup>, and ecosystem sciences samples<sup>31</sup>. The Internet of Samples (iSamples) project used and built upon this crosswalk comparison to identify commonalities and develop a schema for core sample metadata across disciplines<sup>10</sup>.

Metadata about physical samples (such as sample type, material) and their collection details (such as geographic location, collection date) provide information needed for sample discovery, and potential integration and reuse. For example, the BioSample database maintained by the <u>National Center for Biotechnology Information</u> (NCBI) contains records with information and metadata describing the physical materials from which the sequence information stored in other NCBI databases like GenBank are derived<sup>25</sup>. Implementation of standard metadata practices has enabled search and access to genetic sequence data in GenBank since 1979<sup>32</sup> and aggregated species occurrence records in GBIF starting in 2001<sup>33</sup>. As of October 2023, GenBank included over 3.7 billion nucleotide sequences for 557,000 formally described species<sup>34</sup>, and as of February 2025 there are close to 3.1 billion species occurrence records in GBIF that enable a wide variety of synthesis studies. The System for Earth and Extraterrestrial Sample Registration (SESAR)<sup>29,30</sup> contains metadata records for >5 million samples including rock, mineral, sediment, and soil samples; rock, sediment, and ice cores; as well as samples of volcanic gas, fluids (e.g., seawater, river water, hydrothermal fluids), and biological specimens collected as part of Earth, planetary and environmental sciences research.

We found that disciplinary data repositories often provide information on sample metadata templates or requirements, while generalist data repositories, journal publishers, and U.S. agencies often do not provide such guidance (<u>Supplemental Table 1</u>).

#### Sample Identification

Persistent identifiers (PIDs) are globally unique strings, associated with standard metadata, and are resolvable, with "links that continue to provide access [to a digital object or file] into the indefinite future"<sup>35</sup>. PIDs identifying a variety of digital objects have enabled (meta)data sharing, integration and reuse across domains, including cultural heritage<sup>36</sup>, scholarly communication<sup>37,38</sup>, and the natural sciences<sup>19,39</sup>. The use of PIDs is preferable over nonresolvable identifiers, such as <u>Universally Unique IDs (UUIDs)</u> and <u>Darwin Core Triplets</u>, which are commonly used for biological specimens in natural history collections. While these can be modified into a resolvable PID with a URL, they must then be associated with standard metadata and maintained by an institution committed to long-term preservation. Nonresolvable identifiers often contain errors and duplicates and are ineffective for linking related data<sup>22</sup>. The increased use of sample PIDs is an essential component to enable more effective tools for sample tracking and citation.

Within the Earth and environmental sciences, standard practices and tools for assigning PIDs to samples have been in place for decades and enable access, integration, and reuse of high-value (meta)data. The International Generic Sample Number (IGSN) IDs, and other sample PIDs<sup>40</sup> must be managed by organizations committed to long-term sample and (meta)data preservation<sup>41,42</sup>. Though the IGSN ID was originally established in 2004 for Earth science samples, its use has since expanded to include a wide range of interdisciplinary samples<sup>19,41,43-45</sup>. Over 12.5 million IGSN IDs have been created across allocating agents<sup>46</sup>. Major organizations such as the National geological surveys of the US, UK, Australia, South Korea, and Germany also use IGSN IDs for their collections.

Organizations within the biodiversity research community are also increasingly using PIDs for physical specimens and/or digital representations of specimens in order to track use of samples and associated research products. For example, member organizations within the Consortium of European Taxonomic Facilities (CETAF), have implemented CETAF stable identifiers for specimens. These are URI-based identifiers directing humans to a web page about the specimen and computers to a machine-readable, RDF-encoded metadata record<sup>47</sup>. The Distributed System of Scientific Collections (DiSSCo) is a research infrastructure for 200+ European natural science collections that recently began implementing services to provide PIDs for online digital representations of specimens. These digital specimen records act as complementary online surrogates for physical specimens in natural science collections that can be updated to link physical specimens/samples to associated data as it is published over time<sup>48,49</sup>.

Particularly in interdisciplinary ecological studies, Earth science samples collected in the field may be associated with microbial and other omics (genomics, metagenomics, metabolomics) analyses. Microbiologists will typically refer to an isolate by a strain identifier (e.g., "Kra1") or by equivalent prefixed culture collection accession numbers (e.g., ATCC 35583, DSM 2078, JCM 9277)<sup>50</sup>. These are not globally unique and can lead to ambiguity in the literature and public databases, limiting the utility of these accession numbers in searching, indexing, and provenance tracking. For genomics, this ambiguity is mitigated by the use of BioSample

accession numbers<sup>51</sup>. The potentially rich metadata associated with these identifiers is openly available online, providing information about the source sample, as well as references to additional identifier classes for biological projects, analyses, and sequence data. These accession numbers and associated metadata provide near-ideal unique identifiers that lend themselves to efficient retrieval and literature search, though hierarchy concerns and indexing gaps limit their use in generating citation metrics.

#### Publishing Samples and Associated (Meta)Data

There are general requirements now in place from funding agencies to publish all data associated with scientific publications<sup>52</sup> (see Supplemental Table 1). Most journals now have data availability statements and increasingly require that data be published upon submission<sup>53</sup> (https://www.nature.com/nature-portfolio/editorial-policies/reporting-standards). However, few organizations provide explicit guidance on *how to* create and publish datasets associated with samples, and connect samples to downstream data. We found that even for organizations that recommend using sample PIDs and assigning standard metadata, explicit guidance on publishing downstream data and using their sample PIDs throughout the sample data lifecycle was usually lacking (Supplemental Table 1). One exception is the Interdisciplinary Earth Data Alliance (IEDA2), which enables sample identifier hierarchies with parent/child relationships, and for users to provide IGSN IDs associated with their dataset (Supplemental Table 1).

Biodiversity science and genomics are generally further along in providing infrastructure for publishing and connecting standardized sample metadata and associated data. In GBIF, occurrence records can be part of datasets, but records in GBIF are published at an institution-level, not by individual researchers publishing their data (note: datasets in GBIF are often whole natural history collections)<sup>54</sup>. While GBIF now recommends use of sample/specimen PIDs, they do not require them. Other infrastructure in the biodiversity research community connect specimens or digital specimens and downstream research products using XML-based data exchange standards and/or Resource Description Framework (RDF). RDF is a general framework for representing interconnected data on the web (Supplemental Table 1), commonly serialized using JSON-LD for data interchange. NCBI and other International Nucleotide Sequence Database Collaboration (INSDC) databases connect related sample data using identifier hierarchies, BioProject, BioSample, Sequencing Read Archive (SRA), and LinkOut services to connect to other related resources.

#### Sample Citation Practices

Despite decades of PID infrastructure development and sample metadata standards development, there are no consistent recommendations across disciplines for citing samples and associated data, and attribution practices (or lack thereof) vary. To clarify sample citation, we mean referencing sample PIDs in a structured, clearly accessible way within paper text (methods section, within relevant tables, in the data availability statement), in the reference list, and/or within associated dataset metadata and data files. Note that a full citation in a paper should include adding a formal citation in the references list<sup>55</sup>; however, this does not work for

many use cases involving large numbers of samples, as addressed in later sections. In such cases, we can explore practical sample citation practices that make associated studies more FAIR and enable alternative options to track sample use, such as text mining tools<sup>56</sup> or an emerging approach developed in the Research Data Alliance (RDA) Complex Citations Working group that would enable citing large numbers of entities<sup>57</sup>.

Many physical sample repositories and natural history collections request acknowledgement when their samples are used, but practices vary, and many are not sufficient to enable the tracking of individual sample use<sup>58</sup>. Each institution recommends a distinct practice, which often includes museum catalog numbers and the institution name; PIDs may or may not be required. The Field Museum in Chicago, for example, requests that specimens or objects be cited in their preferred format: [occurrenceID].[catalogNumber].[data publisher]<sup>59</sup>. The citation formats for museum collections at the <u>Smithsonian National Museum of Natural History</u> and the <u>American Museum of Natural History (AMNH)</u> are dependent on the division or department under their loan policies<sup>60,61</sup>. For example, the <u>Smithsonian Mineral Sciences</u> collection requires users to cite their collections based on what is available: catalog number, EZID, IGSN ID<sup>62</sup>. The <u>AMNH</u> <u>Paleontology department</u> requires a copy of the manuscript for records and catalog citation<sup>63</sup>.

This variation in recommended citations within and across disciplines results in even greater variations in how authors actually acknowledge long-term collections and samples used, if they do so at all. For example, authors will often mention sample repositories in the Acknowledgments section of a paper, and list individual sample names on a map or table shared as supplemental materials<sup>64</sup>. In both cases, the identifiers may be inconsistently abbreviated with no information about the current archives where the physical samples are held, which is important if the samples need to be accessed and re-analyzed. This reduces the reproducibility of the study, inhibits sample reuse, and makes automated identification or digital scraping of sample citations very difficult or even impossible.

#### Ethics and the CARE Principles for Samples and Associated (Meta)Data

We recognize that not all data derived from samples can be fully open. Cyberinfrastructure designed to share sample metadata must also be designed to protect sensitive data, in particular sensitive sample locations. Samples that are sensitive and/or restricted must be protected through appropriate access controls and have any restrictions documented (such as permits, ethics agreements, access moratoriums). The decision as to whether certain samples and derived data can be made public is not necessarily that of the researcher. For example, the Nagoya Protocol addresses 'Access to Genetic Resources and the Fair and Equitable Sharing of Benefits Arising from their Utilization to the Convention on Biological Diversity'<sup>65</sup>.

When collecting and managing samples related to Indigenous Peoples and their lands and waters, authors should consult the CARE Principles for Indigenous Data Governance<sup>21</sup>. The CARE Principles were developed by Indigenous Peoples, scholars, nonprofit organizations, and governments to address concerns about the secondary use of samples and data derived from these samples collected on their lands. The CARE Principles, which complement the FAIR

Principles<sup>66</sup>, aim to 1) respect Indigenous data sovereignty, and 2) support open data, including secondary use<sup>21,67</sup>. For future sample acquisition, it is essential that the relevant Indigenous communities are engaged prior to any samples being collected, and that wherever possible, local knowledge is included in the collection process to avoid incidents such as the unauthorized sampling of Bishop Tuff in California and other cases elsewhere<sup>68</sup>. Operationalization of the CARE Principles by publishers, data repositories, and researchers is just beginning. Metadata guidance, such as the Indigenous Metadata Bundle Communiqué<sup>69</sup> is important to incorporate in future development of sample metadata standards<sup>70,71</sup>.

# Methods

ESIP is a 501(c)(3) nonprofit supported by NASA, NOAA, USGS, and 130+ member organizations, providing leadership in promoting the collection, stewardship, and use of Earth science data, information, and knowledge. This includes about 30 <u>collaboration areas</u> where members meet regularly to work together on common data challenges. The Physical Samples Curation Cluster is one such group that we organized in January 2021 to promote the discovery, access, and use of physical samples and associated data. Members and our target community include researchers who collect/identify/analyze/use samples and related data products, professionals who manage samples in physical collections, data repository managers, and other cyberinfrastructure providers who support tools and services for physical samples. This includes subject-matter experts from universities, federal organizations such as the U.S. Geological Survey, NASA, NOAA, US Department of Energy, major U.S. scientific sample repositories such as the USGS Core Research Center and the Oregon State University Marine and Geology Repository, data repositories such the Interdisciplinary Earth Data Alliance and the ESS-DIVE data repository, and the international IGSN e.V.

The working group started with the goal of addressing social and technical needs for tracking and publishing sample-related research across scientific disciplines.

### Use Cases for Tracking Sample Use

In group discussions, we identified specific use cases that demonstrated common needs across disciplines for tracking samples to better support sample and data management, data synthesis, and appropriate credit for researchers and institutions. We then outlined real use cases encountered in our work as sample-data experts to inform the final recommendations, including:

- 1. Efficiently publish and cite a large number of samples and associated (meta)data;
- 2. Provide credit for those involved in physical sample collection and curation to demonstrate the value of investing in collections;
- 3. Track the use of sample data generated by analysts and laboratories; and
- 4. Connect related interdisciplinary sample (meta)data and other research outputs.

## Drafting Guidelines Through Community Feedback and Review

Use cases then informed the author guidelines for researchers submitting scientific publications involving physical samples. These guidelines were based on existing best practices <sup>27,42,45</sup> (Supplemental Table 1), use cases that illustrated current challenges and needs, and extensive community feedback and review.

We gathered feedback in regular working meetings and conference sessions. During the monthly meetings, we held discussions, working sessions, and relevant talks on challenges, needs, and visions for publishing and tracking scientific samples and associated data. The group engaged more broadly by convening seven conference sessions at bi-annual ESIP meetings, the 2022 American Geophysical Union meeting, and the Society for the Preservation of Natural History Collections conference. We designed ESIP sessions, in particular, to collect specific feedback through individual reflection (via digital collaborative documents and whiteboards), group discussion, and anonymous poll/survey questions<sup>72,73</sup>. We gathered input from presentations and feedback during group meetings, which informed drafts of the guidelines and improved later versions.

To further refine the guidelines, we coordinated with several related projects and international efforts. This included the <u>Sampling Nature Research Coordination Network</u>, <u>Internet of Samples</u> (iSamples) project<sup>10</sup>, <u>Australian Research Data Commons</u> (ARDC) <u>Information Management for</u> <u>Physical Samples Community of Practice</u>, the RDA <u>Complex Citations Working Group</u>, and the RDA <u>Physical Samples and Collections in the Research Data Ecosystem Interest Group</u>.

We also worked through examples where six different projects, including researchers who had not previously used standard sample identifiers and metadata, applied recommended practices (see Supplemental Information for methods and outcomes).

## Results

### Use Case Review: Needs for Tracking Sample Use

The following use cases informed the final recommendations for scientific authors, journal publishers, data repositories, and indexers, as presented in the results and discussion sections.

# Use Case 1: Efficiently Publish and Cite a Large Number of Samples and Associated (Meta)Data

Many studies that involve physical samples use dozens, hundreds, or even thousands of samples and subsamples. Tracking samples associated with these datasets is important for identifying the impact of samples, particularly for cases where sample collection was expensive or re-sampling is impossible. This includes tracking the full body of knowledge associated with any given sample, and appropriate attribution. There is no widely adopted method to efficiently

cite a large number of datasets<sup>74</sup>, let alone the physical samples linked to them. However, with current infrastructure, metadata describing all samples used in a given dataset can be included. For example, several data repositories currently include sample PIDs as related identifiers in dataset metadata (e.g., <u>EarthChem</u> Library (ECL), <u>Pangaea</u>, and <u>GFZ Data Services</u>).

# A Real-World Example: Connecting Samples and Data in the Interdisciplinary Earth Data Alliance

IEDA2 is a collaborative, NSF-funded data infrastructure that consists of several complementary data systems, including ECL and SESAR. IEDA2 data systems provide services for publishing sample-based analytical datasets using consistent sample metadata and PIDs for samples (IGSN IDs) to unambiguously connect samples and derived data.

SESAR offers IGSN ID registration and management services for researchers and collection curators worldwide, enabling them to permanently store and update sample metadata—including images and links to related datasets and publications—on a persistent and publicly accessible digital sample landing page (e.g., <u>https://doi.org/10.58052/IENHR006K;</u> Figure 1). Researchers may register IGSN IDs by entering metadata for a single sample in a web form, uploading a standardized spreadsheet template for one or more samples, or sending XML-encoded sample metadata from their local sample metadata management system through SESAR's application programming interface (API). SESAR also enables linking related samples (by sites, parent–child samples, and/or sibling samples) by providing parent IGSN ID metadata.

EarthChem provides two distinct, but complementary services: First, it enables access to large volumes of published laboratory analytical data for terrestrial samples (ca. 50 million analytical data points), aggregated and harmonized into synthesis databases with human and machine-actionable interfaces to search and retrieve analysis-ready data<sup>75</sup>. Second, EarthChem enables publishing and archiving datasets in ECL, a FAIR data repository providing standardized data templates for specific disciplines (for example, data derived from volcanic tephra samples<sup>76</sup>). Researchers contributing data to ECL can provide IGSN IDs within a designated column in the data templates and in a distinct metadata field during dataset submission. Upon publication, IGSN IDs are displayed on the dataset landing page, and link to individual IGSN ID sample pages (Figure 1).

As of February 2025, >26% (440) of EarthChem's 1,641 published datasets included links to IGSN IDs, with 34,382 unique IGSN IDs recorded. Within SESAR, ~25,000 publicly-available samples have been linked to EarthChem datasets. This reflects strong community interest and buy-in for a future where these systems have automated links for sample and data discovery, and efforts are underway to develop this through the IEDA2 Geosamples Data Nexus.

#### Summary of Needs

To support efficiently publishing and citing large numbers of samples and associated (meta)data, we suggest the following:

- 1) Authors should use PIDs for their samples, and include them as a column in data files and/or dataset metadata.
- 2) When registering dataset DOIs, data repositories should include sample PIDs as related IDs registered with DataCite.
- 3) Sample metadata and data repositories should enable automatic updates to sample metadata profiles and dataset landing pages as new (meta)data are published. For example, when samples are included in a dataset, the sample landing page should automatically update with a link to that dataset. PIDs must therefore be processed through an indexer or other functional links must exist between pertinent repositories and sample landing pages.
- 4) When a dataset is cited, samples included in that dataset should be automatically recognized and tracked in metrics, for example as addressed in the recommendations of the RDA Complex Citations Working Group<sup>57</sup>.
- 5) Users should be able to easily access sample PIDs and metadata on dataset landing pages; for example, through a weblink or the option to download.

Figure 1 goes here.

### Use Case 2: Provide Credit for Those Involved in Physical Sample Collection and Curation to Demonstrate the Value of Investing in Collections

Tracking sample use is crucial for giving credit to individuals and organizations involved in sample collection and curation, including sample collectors, the repositories and collection managers who curate and manage samples, and funders evaluating impact. For example, physical sample repositories must regularly show the impact of their collections to justify their work and continue to acquire funding. When data and sample stewards are unable to fully document their contributions to science<sup>14</sup> when samples are not cited, collection managers are less able to demonstrate the impact of collections, which, in turn, threatens the sustainability of these valuable scientific assets.

# A Real-World Example: Showing the Impact of the University of Michigan Museum of Zoology

The University of Michigan Museum of Zoology's (<u>UMMZ</u>) <u>Mammal Division</u> manages over 150,000 specimens that are used in a broad range of scientific studies. Each of these specimens has a catalog number—a unique identifier *within the UMMZ* that is associated with both the physical sample and its metadata—but not a PID. To track the use of their collections, staff (led by author CWT) ask researchers who use the collection to include catalog numbers and acknowledge the use of the collections in any subsequent publications. CWT and his team maintain a <u>bibliography in Google Scholar</u> that lists these papers, as well as papers authored by the collection staff and students.

While the publications in the Google Scholar bibliography have accrued over 96,000 citations, this is just a heuristic of specimen use. Because papers *by* the collection staff are mixed with papers *using* the collection, it does not show the impact of specific specimens over time and, therefore, does not precisely show the impact of collections management. To address this, authors [SL, ERC, KF, RN, CWT, AKT<sup>77</sup>] used text mining to extract catalog numbers and generate metrics of use. The results were underwhelming: Of 1,297 papers examined, only 245 included catalog numbers. Instead, researchers thanked the collection in the acknowledgments section without citing specimens, listed specimens in supplementary material that could not be effectively identified and mined, or listed other identifiers that were not used by UMMZ (e.g., GenBank IDs).

#### Summary of Needs

To provide credit for physical sample collection and curation, and to demonstrate the value of investing in collections, we need the following:

- Managers of physical collections should explore assigning PIDs to their specimens. While this takes considerable time and effort, it would make it easier to "mine" citations because they are consistently formatted and resolvable to an online metadata catalog.
- 2) When samples have PIDs, the PIDs must be listed in any papers that use the samples. This could be done by listing the PID in the text of the paper, by citing a sample in the references section, or by including sample PIDs in a dataset cited by the paper.
- 3) Publishers, indexers, and data repositories should work together to aggregate and track the use of all PID types. This might mean that publishers recognize and hyperlink sample PIDs in paper text, indexers build new tools to harvest PIDs from papers and datasets, or data repositories take steps to expose sample PIDs to indexers.
- 4) Subsamples taken from a parent sample should be clearly linked to the parent through related identifiers. For example, GenBank records must link to parent/source samples (ideally with the sample PID) when relevant.

#### Use Case 3: Track the Use of Sample Data Generated from Laboratories

Similar to the sample collectors and physical collections described in Use Case 2, laboratories conducting analyses on samples need to be able to demonstrate the value of their work to funders. Understanding how data are reused is also essential for identifying service improvements that can benefit the laboratories themselves and the communities they serve; for example, focusing on thematic areas that are heavily cited, improving the efficiency of laboratory processes, or allocating resources toward products and services with high-impact potential. However, a laboratory that publishes data or provides samples loses control over provenance information (records of how the sample and data are used) as soon as it ends up in the hands of a third party. Approaches that accumulate metadata in a consistent manner across systems and preserve full provenance information for samples and any derived data are greatly needed.

#### Real-World Example: Citations for Data Generated by the Joint Genome Institute (JGI)

The JGI provides integrated high-throughput sequencing of samples, DNA design and synthesis, metabolomics, and computational analysis. To track its impact on scientific research,

JGI developed the Data Citation Explorer<sup>56</sup>, a web service that identifies the use of genomic data products in published literature even in instances where those products are not properly cited. The service employs heuristics to discover occurrences of unique identifiers associated with genomic data in the text and reconstructs graphs that restore many of the missing connections among these related classes of identifiers. The Data Citation Explorer has been able to identify around 4,000 publications citing JGI data using NCBI identifiers or other standard identifier types. However, concurrent manual expert analyses identified that most researchers cite publications associated with datasets produced from samples if they cite anything at all. The authors estimate that there are tens of thousands of such "nonstandard" references to JGI data that cannot yet be identified using automated tools<sup>56</sup>.

#### Summary of Needs

The following would facilitate tracking use of sample data generated by laboratories:

- 1. Researchers should follow consistent guidelines on how samples and associated (meta)data should be cited. Particularly with a rise in interdisciplinary work, it would be beneficial to use and enforce similar practices across disciplines, journals, institutions and funders.
- 2. Scholars, laboratory managers, and others who register sample identifiers should use PIDs that are globally unique and can be identified and indexed using automated tools.
- Sample metadata and data repositories should use consistent methods of search and retrieval of sample (meta)data (for example, URL formats, API standards, metadata formats), and implement standards to unambiguously link and exchange information for related PIDs<sup>78</sup>.
- 4. Provenance information must be propagated when laboratory and/or sample PIDs are used.

# Use Case 4: Connect Interdisciplinary Sample (Meta)data and Other Research Outputs

Interdisciplinary studies that connect diverse data to understand multiscale processes often involve sample data. These highly related data may be analyzed and published separately on multiple data systems across disciplines, creating a challenge to connect subsamples and data types from the same samples. Future researchers attempting to find and reuse such data often have no way of tracking sample provenance without contacting the authors. These combined challenges make data synthesis involving interdisciplinary samples very difficult.

Real-World Example: Biogeochemical Samples from Projects of the United States Department of Energy's Biological and Environmental Research Program (U.S. DOE BER)

The U.S. DOE BER program is highly interdisciplinary, and samples from its projects are often used to enhance models and predictions of ecological processes and biogeochemical responses to ecosystem disturbances. Scientists on these projects have faced sample tracking challenges due to inefficiencies in the processes of submitting samples to different data systems

and laboratories and then compiling the resulting data. One such project, the <u>River Corridor</u> <u>Hydro-biogeochemistry Science Focus Area</u>, studies hydrologic, biogeochemical, and microbial function within river corridors<sup>79</sup>. Researchers collected a series of individual surface water samples (e.g., <u>https://doi.org/10.58052/IEWDR00RT</u>), sediment samples (e.g., <u>https://doi.org/10.58052/IEWDR0149</u>), and filter samples (e.g.,

https://doi.org/10.58052/IEWDR00UI) at almost 100 global sites (e.g.,

https://doi.org/10.58052/IEWDR00P4) as part of the Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS). DNA and RNA material were extracted from the filter and sediment samples (subsamples/child samples; e.g., https://doi.org/10.58052/IEWDR00UI, and sent to the JGI for metagenomic and metatranscriptomic sequencing. Water and sediment samples were also sent to the Environmental Molecular Sciences Laboratory (EMSL) for metabolomics analyses (Figure 2). They created sample sets and documented their workflows in the DOE Systems Biology Knowledgebase (KBase) and registered an associated study on the National Microbiome Data Collaborative (NMDC) portal

(https://data.microbiomedata.org/details/study/nmdc:sty-11-5tgfr349) as a part of the Genome Resolved Open Watersheds database (GROWdb) effort<sup>80</sup>. NMDC enables easy access to distributed microbiome and related data. In addition, NMDC enables submitting and storing sample metadata in the MIxS standard format for describing contextual information on sampling and sequencing of genomic material. Analysis and visualizations from the sample set were incorporated into formally published datasets for long-term preservation and documentation in the Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) data repository<sup>81,82</sup>. These datasets were then referenced in the final journal publications associated with the data<sup>79,83–85</sup>.

The process of submitting the associated data to multiple systems and adding links and other information as new (meta)data are generated is currently inefficient. The more recently developed NMDC portal has made significant progress, currently enabling centralized submission of standardized sample metadata for microbiome research to JGI and EMSL. And the five BER data systems are working toward developing a more deeply integrated data ecosystem, including automated metadata exchange and enabling global search across systems.

Figure 2 goes here.

#### Summary of Needs

To efficiently connect interdisciplinary sample (meta)data and other research outputs, we need the following:

- 1. Researchers should use sample PIDs for any Earth and environmental source/parent samples and subsamples sent to laboratories.
- 2. (Meta)data repositories and laboratories should promote or provide field apps and other tools for automated registration of sample PIDs with standard metadata at the time of collection/creation of the sample, or soon after, and upon sending subsamples to

different laboratories and user facilities (automatically creating resource maps that specify and display sample relationships).

- 3. Laboratories and data systems should provide tools that map varying, but similar, metadata requirements across different systems<sup>86</sup>.
- 4. (Meta)data repositories and data systems should develop programmatic interfaces or APIs to automatically connect and exchange (meta)data using sample PIDs. For example, automatically cross-link across data systems as new (meta)data are generated, and develop systems for tracking sample use and citations as new (meta)data are published and (re)used over time<sup>87</sup>.
- 5. Relevant data systems should coordinate to better integrate samples and associated data across projects and data systems.

# Recommended Practices for Scientists Publishing Sample-Based Research

The final guidance document, "Publishing Open Research Using Physical Samples: Guidance for Authors", includes foundational elements to make samples and associated (meta)data Open and FAIR<sup>88</sup>. Adoption of this guidance would help to track sample usage over time, which in turn supports reproducible research, data integration, reuse, and credit. The full guidance document includes links to specific examples and additional information on why each step is needed. We have also condensed the guidelines for community distribution within the Earth sciences. These guidelines can be used directly by individual researchers, journal publishers, or data repositories, and can be modified to provide more targeted instructions for specific communities.

A summary of key elements of the full scientific author guide for publishing Open and FAIR research using physical samples<sup>88</sup> include the following:

#### Step 1. Describe Samples with Rich Metadata

Describe key characteristics and collection details of samples in a study using a domain-specific standard or reporting format relevant to your sample type<sup>25,27–30</sup>. This usually involves creating a sample metadata file using a standard template. Specific key metadata fields include sample type, how and where it was collected, by whom, and where it is archived (if applicable). This file is then used to register sample PIDs (Step 2), or is included in relevant datasets (Step 3).

#### Step 2. Assign and/or Use Identifiers for Samples

Assign and/or use existing sample PIDs to track samples and associated data; some institutions or data systems may assign sample PIDs for you. The guidance document provides details for how to assign PIDs in different scenarios.

#### Step 3. Publish and Cite Samples in Datasets

Publish a dataset that includes your sample PIDs and associated data; see <u>existing guidance</u> on how and where to publish datasets. If your samples have PIDs, include them in your dataset(s) metadata, and include a sample PID column (such as column header "IGSN" or "Sample PID") within all data files containing sample data. If your samples do not have PIDs associated with standard metadata, also include a sample metadata file that clearly describes all sample collection details (Step 1) as part of your dataset. Then cite the dataset in the reference section of your paper and include it in your <u>data availability statement<sup>89</sup></u>.

#### Step 4. Cite Sample Identifiers in Paper

If referring to samples within the text and/or table(s) of your paper, use sample PIDs in a consistent standard format to address methods or findings. This includes a prefix identifying the PID type before the number, and a hyperlink to the sample landing page (for example, <u>igsn:10.58052/IEGRW002B</u>) or the full URL (<u>https://doi.org/10.58052/IEGRW002B</u>, depending on journal requirements. This will make your PID findable by both humans and computers.

Note that for valuable samples archived in collections, you should cite sample PIDs in the text or references section where possible. However, when using large numbers of samples, you can cite a dataset that in turn cites the individual samples included (Step 3).

See Supplemental Information for details on how we applied these recommended practices in the ESS-DIVE data repository.

## Discussion

The author's guide for publishing sample-based research (summarized above) is one step toward enabling physical sample discovery, tracking, and attribution. However, author guidelines alone are not enough. There are multiple ways in which scientists, repositories, PID organizations, publishers, and citation indexers can further develop the physical sample research ecosystem (Figure 3), including:

- 1) Promote and incentivize adoption of standard practices;
- 2) Research institutions, physical collections, and laboratories facilitate use of PIDs;
- 3) Implement clear guidelines and editorial review for publishing and citing sample-based research;
- 4) Implement standards for connecting samples and datasets to related outputs;
- 5) Improve citation metrics and provenance tracking; and
- 6) Coordinate across systems to enable automated (meta)data exchange and global sample search.

Figure 3 goes here.

## Promote and Incentivize Adoption of Standard Practices

One of the biggest obstacles to supporting sample tracking and citation is cultural; while there is growing awareness of the need to describe and cite samples used in research, it is not yet the norm for most scientists to do so. Scientists may not be aware of the possibility and benefits of citing PIDs, and lacking incentives otherwise, they follow disciplinary traditions. We need to promote the best practices for publishing sample-based research. This involves advancing incentives that encourage researchers to follow recommended practices and tools that make this process easier and rewarding. Such incentives include useful tools for easy sample data submission, integration, and visualization (as demonstrated by resources like GBIF), and sample citation counts or other records of where and how samples and associated data are used<sup>56,90</sup>.

For newly collected samples, PIDs and standard metadata can be effectively assigned in the field at the time of sample collection using automated field apps, such as "Dirt to Desktop"<sup>91</sup> and StraboSpot<sup>92</sup>. These GPS-enabled apps automate the capture of precise geographical coordinates at the time of collection and can be preset to collect a consistent set of metadata attributes for a major field sampling campaign. Not all sampling locations have internet access, but the information can be stored offline and automatically loaded to the home database when an internet connection becomes available<sup>91</sup>. They also remove the chance of transcription errors and save time and money<sup>92</sup>. The IGSN ID, geolocation, time of collection, and other critical metadata are efficiently and consistently captured in the field and are ready to submit on return.

We can promote a culture of sample citation and PID uses by mentoring and training researchers, as well as through funding and journal requirements. Some funders now recommend or require the use of sample PIDs in data management plans, which is an important step. For example, the U.S. NSF GEO Data and Sample Policy request IGSN ID registration through the SESAR<sup>11</sup>. Journals can include guidance for samples in their publication requirements (for example, <u>AGU includes IGSN IDs in their guidance for authors</u>).

# Research Institutions, Physical Collections, and Laboratories Facilitate Use of PIDs

The research institutions, physical collections, and laboratories that manage physical samples have a major role to play in facilitating sample publication, citation, and tracking. PID registration can be more readily incorporated into required (and ideally automated) workflows of these institutions throughout the sample collection and management lifecycle. After source sample PIDs are assigned, researchers from institutions analyzing samples may additionally facilitate sample tracking and citation by minting child PIDs for any subsamples taken from their collections (Figure 3, *1-3*).

Existing services and new technology are lowering barriers for institutions to adopt PIDs and develop local PID allocation services. For 20 years, SESAR has provided curation services and a user-friendly sample registration service for researchers for no fee. The Internet of Sample

(iSamples) project is experimenting with methods of aggregating sample records by serving data from existing local sample PID registration services using a unified metadata profile<sup>10</sup>. DISSCo uses an approach to assign DOIs to the digital records for specimens (not the physical sample itself), which could simplify updating records for large numbers of specimens contributed by different sample collectors/owners, linking to related resources over time, and avoid relabeling physical samples<sup>48,49</sup>. Institutions and researchers have a growing number of options to implement standard sample metadata publication and citation in their research.

# Implement Clear Guidelines and Editorial Review for Publishing and Citing Sample-Based Research

Data repositories and sample metadata repositories can contribute by providing clear guidance and editorial review on identifying, describing, and reporting use of samples in datasets. While many disciplinary repositories already provide guidance on sample IDs and metadata, there is often little guidance for publishing and connecting related data over time (Supplemental Table 1; Figure 3, improvements 4 and 5). Such data repositories can now use or adapt the guidelines developed in this publication and the associated guidance document developed by the ESIP Physical Samples Curation Cluster to address these issues and move toward common practices across systems.

Journal publishers must recognize the role of citations for research products beyond research articles, and require citations for datasets, physical samples, and beyond (improvement 5, Figure 3). Some journal publishers already provide data and software citation guidance<sup>93</sup>; similar author instructions are needed on where and how to cite samples in publications and/or associated datasets. This includes information about how to encode sample PIDs so that they become linked in the publication process (Figure 3, Improvements 7-8). This guidance should outline procedures for all components of a paper (how to cite sample PIDs in line in text, in tables, and how they should appear in Data Availability statements or reference sections) or a dataset where relevant. During the review process, journal and data editors should ensure that PIDs are formatted in a way that they can be easily indexed and are reliably linked to related metadata records.

# Implement Standards for Connecting Samples and Datasets to Related Research Outputs

Sample PIDs and standard metadata are the foundational elements necessary to track and update provenance information. Some data repositories have systems in place for connecting datasets to related entities through, for example, provenance metadata, the RDF metadata framework for exchanging information, and/or DataCite metadata schema ("RelatedIdentifier", and "RelationType" fields; Supplemental Table 1)<sup>94</sup>; many of these approaches could be extended to relate samples to their data and publications. However, many data archives do not have dataset metadata fields specifically for samples and other related identifiers. We

recommend that data repositories store related sample identifiers in their datasets' metadata (Figure 3, Improvement 6). Currently, the benefit of using the DataCite metadata is that their "RelatedIdentifier" and "RelationType" fields are used by DataCite to track citations to datasets and related works more easily, and thereby better show the impact of data (<u>https://support.datacite.org/docs/connecting-to-works</u>)<sup>94</sup>. Data repositories serving sample-based research should further provide the functionality to recognize sample PIDs as related entities associated with and cited by the dataset. For example, EarthChem automatically extracts IGSN IDs from data files and clearly displays links to the samples on the dataset landing page (for example, <u>https://doi.org/10.26022/IEDA/112300</u>).

Sample PIDs should generally be linked to other identifiers using defined relationship types, such as DataCite metadata described above<sup>94</sup>. This includes other samples with PIDs (parent-subsample as "IsPartOf", or parent–child as "IsDerivedFrom"), and datasets that include sample (dataset DOI "HasPart" and "References" sample DOI/IGSN ID). Connecting sample PIDs to all downstream sample/research products enables indexers to automatically create and track directional linkages. Furthermore, we need to make these related identifiers agnostic to identifier type, going beyond DOIs to include the range of identifiers in use, such as <u>ARKs</u>, BioSample Accession numbers<sup>51,95</sup>, and more.

#### Improve Citation Metrics and Provenance Tracking

Citation metrics work fairly well for journal publications and researchers, but improvements are needed for data and sample citation<sup>55</sup>. Indexers that currently provide paper and data citation metrics, such as CrossRef and DataCite, need to consistently recognize sample PIDs as entities in citation metrics (currently only IGSN IDs/sample DOIs are tracked; Figure 3, Improvement 9). Further, at the present time, metrics and usage tracking are only available for DOIs (which include IGSN IDs). We need metrics and usage tracking to be implemented for a range of identifiers in order to make sample-based research truly open and FAIR. Existing initiatives, such as the Make Data Count effort, are working toward making data citation work more consistently<sup>96</sup>.

All institutions involved in the sample collection and data and metadata lifecycle can contribute to a network of related identifiers that links (meta)data across PID registries and related research outputs. If sample PIDs and related identifiers are captured in parent-child sample records and dataset metadata, we can design APIs to efficiently cross-link and exchange information where needed across sample repositories, data repositories, journals, and more when sample PIDs are cited. This will make it possible to track the use of samples and attribute appropriate credit to those involved in sample collection, management, and analysis, as well as document provenance and relationships that make samples and associated data more useful. Tracking sample use will often require traversing multiple links in a graph of related PIDs. For example, this may involve a paper citing a dataset, the dataset citing analyses done on subsamples, and subsamples citing the original source sample collected in the field and/or

archived in a museum. Currently, there are few effective ways of doing this traversal, making it challenging to track sample usage *en masse*.

We need a new approach to effectively recognize sample citations. The <u>RDA Complex Citation</u> <u>Working Group</u>, has outlined needs across multiple use cases to enable citing large numbers of objects (that may originate across multiple data systems) in a single container citation<sup>57</sup>. One of the key use cases for complex citations is to make it possible for authors to cite as many samples as needed in a paper or dataset in a machine-readable way, with the goal of enabling both provenance tracking and credit. Indexers then need to actually harvest those citations accurately from datasets and journal articles<sup>57</sup>.

### Coordinate Across Systems to Enable Automated Metadata Exchange and Global Sample Search

Sample metadata repositories and data repositories are often siloed and need better integration across one another, as well as connections to journal publishers. For example, many IGSN ID Allocating Agents are specific to a country, discipline, or organization and store richer metadata than that which is shared via DataCite when registering samples for IGSN IDs. Though <u>DataCite</u> <u>Commons</u> now enables searching for samples across all IGSN allocating agents, search is limited to this high-level DataCite metadata, and researchers must visit multiple systems to find more detailed sample metadata. Additionally, these distributed services are often not connected to other key systems where associated metadata and data are added over time, such as laboratories, data repositories, and journal publishers. The sample PIDs could be far more valuable to researchers with tools to automatically cross-link, update, and exchange information about samples over time (improvements 6, 8, and 9, Figure 3).

Sample metadata repositories, data repositories, journals, and indexers must coordinate to implement community practices and technical solutions that enable automated linking and information exchange described above, which can apply to samples or any other PID used. Groups such as the <u>ESIP Physical Sample Curation Cluster</u> (including many of the authors of this paper), the Research Data Alliance (RDA) Physical Samples and Collections in the <u>Research Data Ecosystem</u>, RDA Coordinating Earth, Space, and Environmental Science Data <u>Preservation and Scholarly Publication Processes Working Group</u>, and the <u>Coalition for Publishing Data in the Earth and Space Sciences (COPDESS)</u> can help promote and facilitate such coordination.

There are also emergent infrastructure development projects that aim to bridge these silos. For example, the iSamples project aims to build connections across distributed sample metadata catalogs by aggregating sample metadata into iSamples Central<sup>10</sup>. This aggregation means that researchers would only need to search for samples in one place, rather than in multiple repositories. Additionally, several US federal agencies have plans to develop federated systems allowing discovery and access to federally-funded data and articles (See: NSF National Center

for Atmospheric Research<sup>97</sup>). There is generally a push toward 'open research commons' within geoscience and more broadly. These important efforts should include samples and associated (meta)data as a major component.

### Advancing Physical Sample-Based Research

Scientists and sample managers face similar challenges with regard to sample use tracking across specific use cases and disciplines. We believe that this limited set of community practices and improved infrastructure can solve many current challenges, and make it possible to create useful tools for sample discovery, visualization, integration and reuse. Standard practices and improved infrastructure can also make it easier to find and access materials that no longer exist outside of a museum, or are no longer available to be sampled, which saves time and money and enables science that would not be possible otherwise<sup>98</sup>. For example, new studies are published using GBIF records every day, addressing topics such as conservation, species distribution, climate change impacts, macroecological patterns, and more<sup>9,99</sup>. Similarly, the reuse of genomics datasets has contributed to research with diverse applications, for example in the industrial biotechnology<sup>100</sup> and biomedical<sup>101</sup> sectors, and has enabled researchers to better understand the biological effects of ecosystem disturbance<sup>102</sup>. We can advance other environmental science and interdisciplinary studies with more widespread use of standard practices and improvements to infrastructure.

We have described the need for sample and associated data publication and citation guidelines, cultural changes, and infrastructure development to better facilitate physical sample discovery, citation, and tracking. Through years of iterative development, we created author guidelines for sample publication and citation as one step toward this vision. Data repositories and journals can now use and adapt the author guidelines developed by the ESIP Physical Samples Curation Cluster to provide clear guidance for authors submitting data and journal publications<sup>88</sup>. A key element of these recommendations is the wide implementation and adoption of the Sample PID, which provides a powerful way to link and exchange relevant scientific information across facilities and data systems. Overall, these guidelines would enable future development of automated tools to track sample use over time while making samples and associated data Open and FAIR.

### Acronyms

Abbreviation	Name and link to more information
AMNH	American Museum of Natural History
API	Application Programming Interface
ARDC	Australian Research Data Commons
ARK	Archival Resource Key identifier

Table 3. List of acronyms used throughout the paper with links to more information.

BER	Office of Biological and Environmental Research
CARE	Collective Action, Authority to Control, Responsibility, and Ethics
COPDESS	Coalition for Publishing Data in the Earth and Space Sciences
U.S. DOE	United States Department of Energy
DOI	Digital Object Identifier
EAR	NSF Division of Earth Sciences
ECL	Earthchem Library
EMSL	Environmental Molecular Sciences Laboratory
ESIP	Earth Science Information Partners
ESS	Environmental System Science Program
ESS-DIVE	Environmental System Science Data Infrastructure for a Virtual Ecosystem
EZID	University of California Identifiers Service
FAIR	Findability, Accessibility, Interoperability, and Reusability
GBIF	Global Biodiversity Information Facility
GFZ	<u>German Research Centre for</u> <u>Geosciences (GeoForschungsZentrum)</u>
ID	Identifier
IEDA2	Interdisciplinary Earth Data Alliance
IGSN e.V.	IGSN Implementation Organization
IGSN ID	International Generic Sample Number
iSamples	Internet of Samples
JGI	Joint Genome Institute
JGI GOLD	<u>Joint Genome Institute Genomes OnLine</u> <u>Database</u>
KBase	Department of Energy Systems Biology Knowledgebase
LBNL	Lawrence Berkeley National Laboratory
LIMS	Laboratory Information Management System

LLNL	Lawrence Livermore National Laboratory
ORCiD	Open Researcher and Contributor ID
NASA	National Aeronautics and Space Administration
NCBI	National Center for Biotechnology
NMDC	National Microbiome Data Collaborative
NOAA	National Oceanic and Atmospheric Administration
NSF	National Science Foundation
PID	Persistent Identifier
PNNL	Pacific Northwest National Laboratory
RDA	Research Data Alliance
SESAR	System for Earth and Extraterrestrial Registration
UMMZ	University of Michigan Museum of Zoology
URL	Uniform Resource Locator
USGS	United States Geological Survey
UUID	Universally Unique Identifier

## Data Availability

The resulting "Scientific Author Guide for Publishing Open Research Using Physical Samples," as well as relevant community meeting presentations are available in the <u>ESIP Figshare</u> research repository<sup>72,73,88,103</sup>.

The <u>ESS-DIVE data repository</u> has 29 datasets (as of February 2025) compiled into a data portal <u>collection for Environmental System Science samples</u>, which generally include IGSN IDs and standard metadata for associated samples. This includes 10 datasets with detailed links to related samples and other research outputs<sup>69,70,81,82,104–111</sup>.

## Code Availability

No new code was generated in this work.

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# Figures



**Figure 1.** Diagram depicting linkages between ECL (<u>https://doi.org/10.26022/IEDA/112300</u>) and SESAR. a) During dataset submission, authors are provided with a dedicated PID metadata field to provide sample PIDs. Once the dataset is submitted, the system verifies and hyperlinks the PIDs (in this case IGSN IDs). b) Linked IGSN IDs lead to a permanent, publicly available metadata "landing page." For the sample shown, additional subsample ("child") IGSN IDs have been registered and are linked. The IGSN ID registrant has provided the DOI for the dataset shown in (a) in a dedicated metadata field for related URLs or DOIs. c) A "child" subsample ("siblings"). The IGSN ID registrant has manually provided the DOI for the dataset shown in (a).



**Figure 2.** Tracking and linking one source material sample from the River Corridor Hydro-biogeochemistry Science Focus Area project, based on the iSample relational data model<sup>10</sup> which links related samples based on entities such as project, sampling site, subsamples, as well as other related links.



**Figure 3.** Diagram of the sample-based research ecosystem. Blue arrows represent the exchange of metadata as enabled by physical sample PIDs. Areas in which scientific practices need to improve are indicated by orange symbols, and areas in which technical infrastructure is needed are indicated by red symbols. These improvements (called out with numbers *N*, in the lower left and right corners of triangles) would enable efficient sample and data use tracking, and make sample data more FAIR.

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## **Competing Interests**

The authors declare no competing interests.

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