

Building provenance

Note - It is rare for a dataset to have provenance - though we would like to see that change by encouraging researchers to submit scripts whenever it is reasonable. When processing datasets if you notice that provenance is needed let Daphne or Jeanette know.

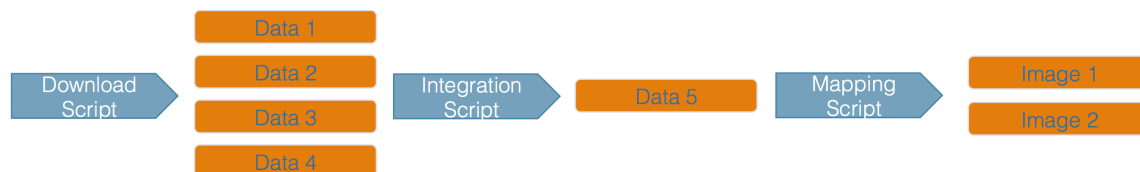
The provenance chain describes the origin and processing history of data. Provenance (or “prov”) can exist on a continuum, ranging from prose descriptions of the history, to formal provenance traces, to fully executable environments. In this section we will describe how to build provenance using formal provenance traces in DataONE.

Provenance is becoming increasingly important in the face of what is being called a reproducibility crisis in science. J. P. A. Ioannidis (2005) wrote that “Most Research Findings Are False for Most Research Designs and for Most Fields”. Ioannidis outlined ways in which the research process has lead to inflated effect sizes and hypothesis tests that codify existing biases.

The first step towards addressing these issues is to be able to evaluate the data, analyses, and models on which conclusions are drawn. Under current practice, this can be difficult because data are typically unavailable, the method sections of papers do not detail the computational approaches used, and analyses and models are often conducted in graphical programs, or, when scripted analyses are employed, the code is not available.

And yet, this is easily remedied. Researchers can achieve computational reproducibility through open science approaches, including straightforward steps for archiving data and code openly along with the scientific workflows describing the provenance of scientific results (e.g., Hampton et al. (2015), Munafò et al. (2017)).

At NCEAS and in the datateam, not only do we archive data and code openly, but we also describe the workflows that involve that data and code using provenance, formalizing the provenance trace for a workflow that might look like this

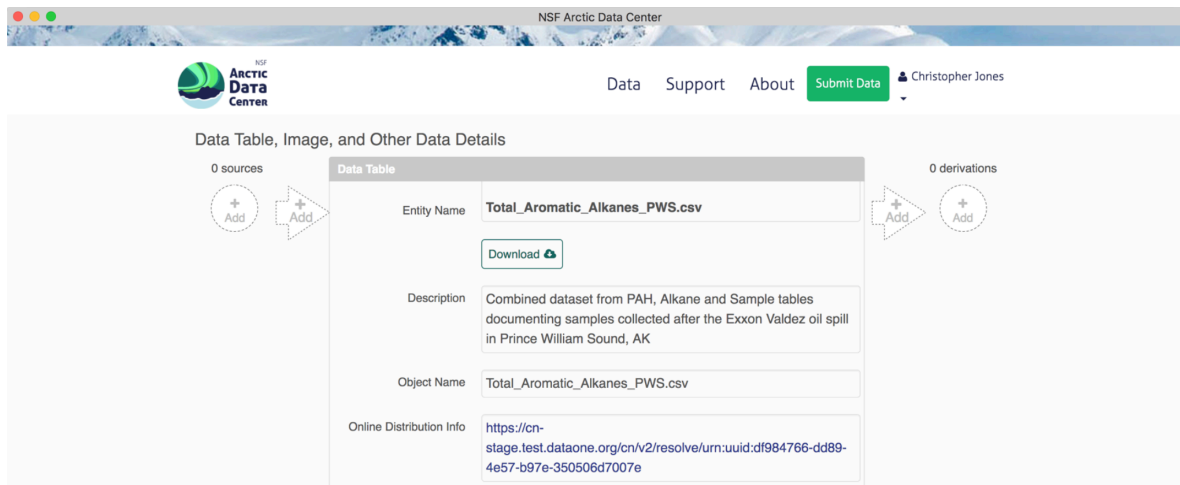


into an easily understandable trace including archived data objects, such as what is shown here.

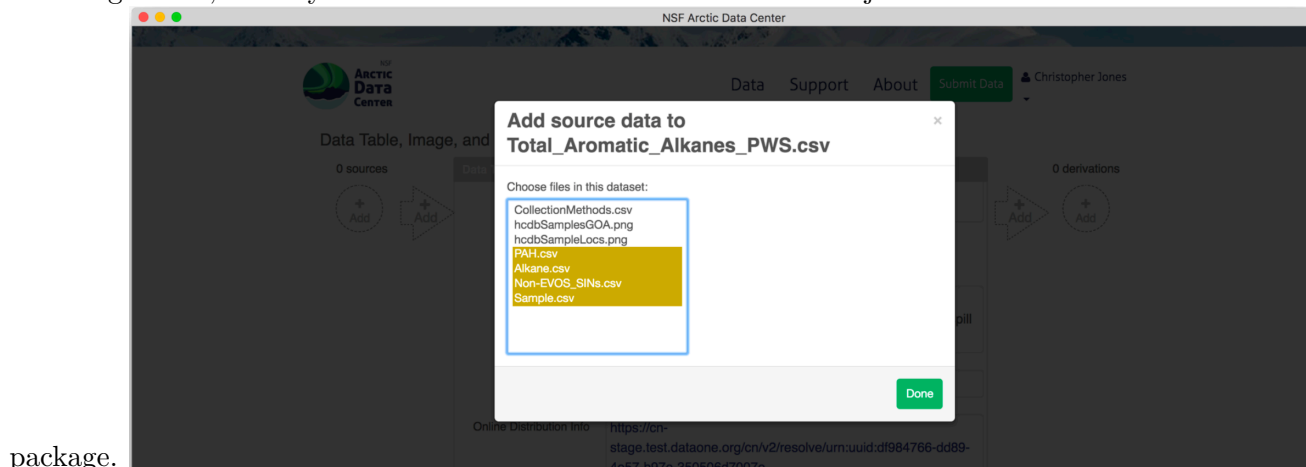
There are two ways that we add provenance in the datateam - the prov editor and the R `datapack` package.

Using the prov editor

Provenance can easily be added to production Arctic Data Center packages using the provenance editor on the Arctic Data Center. On the landing page of a data package within beta, in the **dataTable** or **otherEntity** section where you would like to add a provenance relationship, you can choose to add either a “source” or a “derivation”, to the left or right of the object pane, respectively.

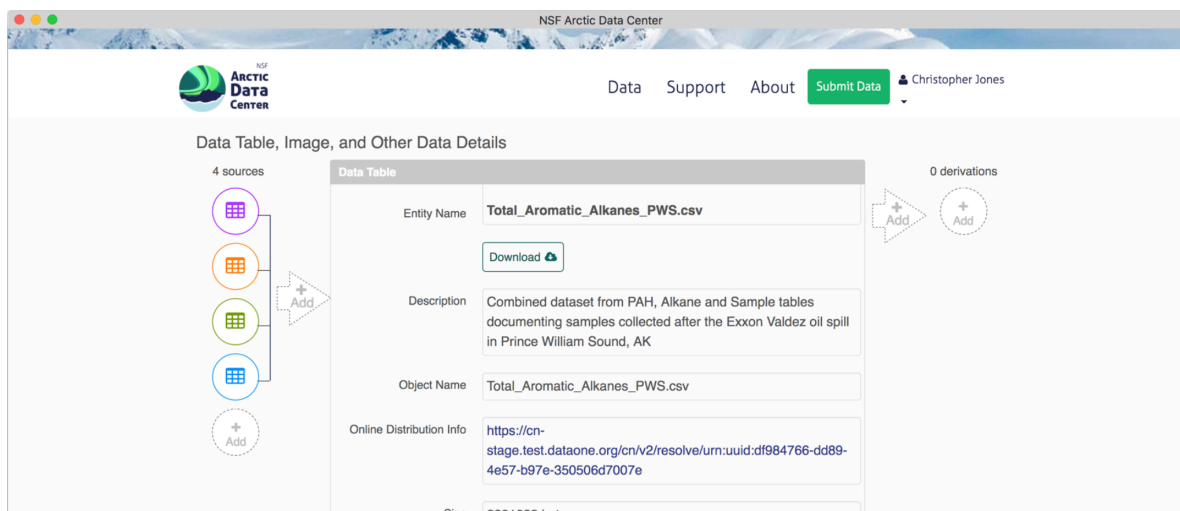


To add a source data file, click on the circle with the “+ add” text. Similarly, a source script would be added by selecting the arrow. Selecting the circle to add a source file pulls up the following screen, where you can select the source from other data objects within the same data



package.

A data package with an object that has multiple sources added will look like this.



For simple packages on the Arctic Data Center, adding prov through the prov editor is super easy!

Understanding resource maps

Before we dive further into constructing prov in R, we need to talk more about resource maps (or “resmaps”).

All data packages have a single resource map. But what is a resource map and how do we use one to find out what objects are in a particular data package? This document is a short introduction but a more complete guide can be found [here](#).

A resource map is a special kind of XML document that describes (among other things) an “aggregation”. The aggregation describes the members of a data package (metadata and data, usually). We can use the `dataone` R package to download a resource map if we know its PID:

```
library(dataone)

d1c_test <- dataone::D1Client("STAGING", "urn:node:mnTestARCTIC")
pid <- "urn:uuid:82bd7d7f-9e18-4fd2-8bda-99b1fddab556" # A resource map PID

path <- tempfile(fileext = ".xml") # We're saving to a temporary file but you can save elsewhere
writeLines(rawToChar(getObject(d1c_test@mn, pid)), path) # Write the object to `path`
```

If we open that file up in a text editor, we see this:

```
<?xml version="1.0" encoding="utf-8"?>
```

```

<rdf:RDF xmlns:cito="http://purl.org/spar/cito/" xmlns:dc="http://purl.org/dc/elements/1.1/"
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A61b48e72-ea2"
    <cito:isDocumentedBy rdf:resource="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3Ac59b7505-39e1"
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A82bd7d7f-9e1"
    <rdf:type rdf:resource="http://www.openarchives.org/ore/terms/Aggregation"/>
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3Ac59b7505-39e1"
    <cito:isDocumentedBy rdf:resource="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3Ac59b7505-39e1"
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3Ac59b7505-39e1"
    <cito:documents rdf:resource="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A61b48e72-ea2"
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3Ac59b7505-39e1"
    <cito:documents rdf:resource="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3Ac59b7505-39e1"
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A61b48e72-ea2"
    <ore:isAggregatedBy rdf:resource="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A82bd7d7f-9e1"
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A82bd7d7f-9e1"
    <dc:title>DataONE Aggregation</dc:title>
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A82bd7d7f-9e1"
    <dcterms:identifier rdf:datatype="http://www.w3.org/2001/XMLSchema#string">urn:uuid:82bd7d7f-9e1</dcterms:identifier>
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A82bd7d7f-9e1"
    <ore:describes rdf:resource="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A82bd7d7f-9e1"
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3Ac59b7505-39e1"
    <ore:isAggregatedBy rdf:resource="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A82bd7d7f-9e1"
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A82bd7d7f-9e1"
    <ore:aggregates rdf:resource="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A61b48e72-ea2"
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A82bd7d7f-9e1"
    <ore:aggregates rdf:resource="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3Ac59b7505-39e1"
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A82bd7d7f-9e1"
    <rdf:type rdf:resource="http://www.openarchives.org/ore/terms/ResourceMap"/>
  </rdf:Description>
  <rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A61b48e72-ea2"
    <dcterms:identifier rdf:datatype="http://www.w3.org/2001/XMLSchema#string">urn:uuid:61b48e72-ea2</dcterms:identifier>
  </rdf:Description>

```

```
<rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3Ac59b7505-39e6-4def-bc82-b67a8d117ce5"
  <dcterms:identifier rdf:datatype="http://www.w3.org/2001/XMLSchema#string">urn:uuid:c59b7505-39e6-4def-bc82-b67a8d117ce5
</rdf:Description>
</rdf:RDF>
```

Whoa! What is this thing and how do you read it to find the members of the data package?
The short answer is to look for lines like this:

```
<rdf:Description rdf:about="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3A82bd7d7f-9e18-4fd2-8bda-99b1fddab556"
  <ore:aggregates rdf:resource="https://cn.dataone.org/cn/v2/resolve/urn%3Auuid%3Ac59b7505-39e6-4def-bc82-b67a8d117ce5"
  </ore:aggregates>
</rdf:Description>
```

This line says “The aggregation aggregates urn:uuid:c59b7505-39e6-4def-bc82-b67a8d117ce5” so that means urn:uuid:c59b7505-39e6-4def-bc82-b67a8d117ce5 is in our data package! The key bit is the `<rdf:Description rdf:about="...#aggregation` part. If you look for another similar statement, you’ll also see that urn:uuid:61b48e72-ea29-4ba5-8131-4f59a9ebcd27 is part of our data package.

Now we know *which* objects are in our data package but we don’t know which one contains metadata and which one contains data. For that, we need to get a copy of the system metadata for each object:

```
getSystemMetadata(d1c_test@mn, "urn:uuid:c59b7505-39e6-4def-bc82-b67a8d117ce5")@formatId
getSystemMetadata(d1c_test@mn, "urn:uuid:61b48e72-ea29-4ba5-8131-4f59a9ebcd27")@formatId
```

From the `formatIds`, we can see the first PID is the EML (`formatId: [1]"eml://ecoinformatics.org/eml-2.1"`) and the second PID is a data object (`formatId: [1]"application/octet-stream"`). Now we know enough to know what’s in the data package:

- Resource map: urn:uuid:82bd7d7f-9e18-4fd2-8bda-99b1fddab556
- Metadata: urn:uuid:c59b7505-39e6-4def-bc82-b67a8d117ce5
- Data: urn:uuid:61b48e72-ea29-4ba5-8131-4f59a9ebcd27

Now that you’ve actually seen a resource map, we can dive further into prov.

Using the datapack package

For packages not on the ADC, or packages that are extremely complicated, it may be best to upload prov relationships using R. The `datapack` package has several functions which help add relationships in a very simple way. These relationships are stored in the resource map. When you update a package to only add prov, the package will not be assigned any new identifiers **with the exception of the resource map**.

First, we set the environment, in a similar, but slightly different way than what you may be used to. Here the function `D1Client()` sets the DataONE client with the coordinating node instance as the first argument, and member node as the second argument.

```
library(dataone)
library(datapack)
d1c <- D1Client("STAGING2", "urn:node:mnTestKNB")
```

Next, get the PID of the resource map of the data package you are adding prov to, and load that package into R using the `getDataPackage()` function.

```
packageId <- "urn:uuid:8f501606-2c13-4454-b22d-050a4176a97b"
dp <- getDataPackage(d1c, id=packageId, lazyLoad=TRUE, limit="OMB", quiet=FALSE)
```

Printing `pkg` in your console shows you the contents of the data package, including all of the objects and their names:

```
> pkg
```

Members:

filename	format	mediaType	size	identifier
esc...er.R	application/R	NA	888	knb.92049.1
PWS....csv	text/csv	NA	1871469	knb.92050.1
PWS....csv	text/csv	NA	1508128	knb.92051.1
NA	eml:/...-2.1.1	NA	15658	urn:uuid:8f501606-2c13-4454-b22d-050a4176a97b

Package identifier: resource_map_urn:uuid:8f501606-2c13-4454-b22d-050a4176a97b

RightsHolder: <http://orcid.org/0000-0002-2192-403X>

It will also show the existing relationships in the resource map, which in this case are mostly the “documents” relationships that specify that the metadata record is describing all of these data files.

Relationships:

	subject	predicate
2	esc_reformatting_PWSweirTower.R	cito:isDocumentedBy urn:uuid:8f501606-...4-b22d-050a4176a97b
4	PWS_weirTower.csv	cito:isDocumentedBy urn:uuid:8f501606-...4-b22d-050a4176a97b
1	PWS_Weir_Tower_export.csv	cito:isDocumentedBy urn:uuid:8f501606-...4-b22d-050a4176a97b
3	urn:uuid:8f501606-...4-b22d-050a4176a97b	dcterms:creator _r151554205
5	urn:uuid:8f501606-...4-b22d-050a4176a97b	cito:documents esc_reformatting_PWSweirTower.R
6	urn:uuid:8f501606-...4-b22d-050a4176a97b	cito:documents PWS_weirTower.csv
7	urn:uuid:8f501606-...4-b22d-050a4176a97b	cito:documents PWS_Weir_Tower_export.csv

```
8 urn:uuid:8f501606-...4-b22d-050a4176a97b      cito:documents urn:uuid:8f501606-...4-b22d-0
9 urn:uuid:8f501606-...4-b22d-050a4176a97b cito:isDocumentedBy urn:uuid:8f501606-...4-b22d-0
```

In this example above, the data package has two .csv files, with an R script that converts one to the other. To create our provenance trace, first we need to select the source object, and save the PID to a variable. We do this using the `selectMember()` function, and we can query part of the system metadata to select the file that we want. This function takes the data package (`pkg`), the name of the `sysmeta` field to query (in this case we use the `fileName`), and the value that you want to match that field to (in this case, 'PWS_Weir_Tower_export.csv').

```
sourceObjId <- selectMember(dp, name="sysmeta@fileName", value='PWS_Weir_Tower_export.csv')
```

This returns a list of the source object PIDs that match the query (in this case only one object matches).

```
> sourceObjId
[1] "knb.92051.1"
```

Now we need to select our output object. Here, we use the `selectMember()` function again, and save the result to a new variable.

```
outputObjId <- selectMember(dp, name="sysmeta@fileName", value='PWS_weirTower.csv')
```

Now we query for the R script. In this case, we query based on the value of the `formatId` as opposed to the `fileName`. This can be useful if you wish to select a large list of PIDs that are all similar.

```
programObjId <- selectMember(dp, name="sysmeta@formatId", value="application/R")
```

Next, you use these lists of PIDs and a function called `describeWorkflow()` to add these relationships to the data package. Note that if you do not have a program in the workflow, or a source file, you can simply leave those arguments blank.

```
dp <- describeWorkflow(dp, sources=sourceObjId, program=programObjId, derivations=outputObjId)
```

Viewing `pkg` again confirms that these relationships have been inserted into the data package, as shown by the `wasDerivedFrom` and `wasGeneratedBy` statements. It is always a good idea to print `pkg` to confirm that your PID selection process worked as expected, and your prov relationships make sense.

Relationships (updated):

	subject	predicate	
15	_1db49d06-ae98-4...9101-39f7c0b45a95	rdf:type	prov:A
14	_1db49d06-ae98-4...9101-39f7c0b45a95	prov:hadPlan	esc_reformatting_PWSw
1	esc_reformatting_PWSweirTower.R	cito:isDocumentedBy	urn:uuid:8f50160...b22d-05
16	esc_reformatting_PWSweirTower.R	rdf:type	provone
8	PWS_weirTower.csv	cito:isDocumentedBy	urn:uuid:8f50160...b22d-05
11	PWS_weirTower.csv	rdf:type	pr
20	PWS_weirTower.csv	prov:wasDerivedFrom	PWS_Weir_Tower_e
19	PWS_weirTower.csv	prov:wasGeneratedBy	urn:uuid:3dd59b0...bc38-3b
6	PWS_Weir_Tower_export.csv	cito:isDocumentedBy	urn:uuid:8f50160...b22d-05
10	PWS_Weir_Tower_export.csv	rdf:type	pr
9	_r1515544826r415842r1	foaf:name	DataONE
17	urn:uuid:3dd59b0...bc38-3b5d8fa644ac	dcterms:identifier	urn:uuid:3dd59b0...bc38-3b
13	urn:uuid:3dd59b0...bc38-3b5d8fa644ac	rdf:type	provone
12	urn:uuid:3dd59b0...bc38-3b5d8fa644ac	prov:qualifiedAssociation	_1db49d06-ae98-4...9101-39
18	urn:uuid:3dd59b0...bc38-3b5d8fa644ac	prov:used	PWS_Weir_Tower_e
5	urn:uuid:8f50160...b22d-050a4176a97b	cito:documents	esc_reformatting_PWSw
4	urn:uuid:8f50160...b22d-050a4176a97b	cito:documents	PWS_weir
3	urn:uuid:8f50160...b22d-050a4176a97b	cito:documents	PWS_Weir_Tower_e
2	urn:uuid:8f50160...b22d-050a4176a97b	cito:documents	urn:uuid:8f50160...b22d-05
7	urn:uuid:8f50160...b22d-050a4176a97b	cito:isDocumentedBy	urn:uuid:8f50160...b22d-05

Finally, you can upload the data package using the `uploadDataPackage()` function, which takes the DataONE client `d1c` we set in the beginning, the updated `pkg` variable, some options for public read, and whether or not informational messages are printed during the upload process. **First, you will need to run a token obtained from <https://dev.nceas.ucsb.edu/> to publish to that node.**

```
resmapId_new <- uploadDataPackage(d1c, dp, public = TRUE, quiet = FALSE)
```

If successful you should be able to navigate to the landing page of your dataset, and icons should show up where the sources and derivations are, such as in this example:

1 inputs

Other Entity

Entity Name:

Download

Data Object Type:

Physical Structure Description:

Object Name:

Size:

Authentication:

Externally Defined Format

Format Name:

Online Distribution Info:

1 outputs

Fixing mistakes

If you messed up updating a data package using `datapack`, there unfortunately isn't a great way to undo your work, as the `describeWorkflow()` only adds prov relationships, it does not replace them. If you messed up, the best course of action is to update the resource map with a clean version that does not have prov using `update_resource_map()`, and then go through the steps outlined above again.

Note: this has not been thoroughly tested, and more extreme actions may be necessary to fully nuke the prov relationships. Consult Peter or Jeanette if things do not work as expected.

References

Ioannidis, John P A. 2005. "Why Most Published Research Findings Are False." *PLoS Medicine* 2 (8): e124. <https://doi.org/10.1371/journal.pmed.0020124>.

Hampton, Stephanie E, Sean Anderson, Sarah C Bagby, Corinna Gries, Xueying Han, Edmund Hart, Matthew B Jones, et al. 2015. "The Tao of Open Science for Ecology." *Ecosphere* 6 (July). <https://doi.org/10.1890/ES14-00402.1>.

Munafò, Marcus R., Brian A. Nosek, Dorothy V. M. Bishop, Katherine S. Button, Christopher D. Chambers, Nathalie Percie du Sert, Uri Simonsohn, Eric-Jan Wagenmakers, Jennifer J.

Ware, and John P. A. Ioannidis. 2017. “A Manifesto for Reproducible Science.” *Nature Human Behaviour* 1 (1): 0021. <https://doi.org/10.1038/s41562-016-0021>.