



University of
St Andrews

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Depositing datasets in Pure: when and how

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Website: <https://www.st-andrews.ac.uk/library/services/researchsupport/researchdata/>

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When to deposit

Below is the sequence of steps that we advise you to follow in order to deposit your dataset in Pure and obtain a DOI. See p. 3 for the workflow referenced against the publication process. More details are provided in the following sections.

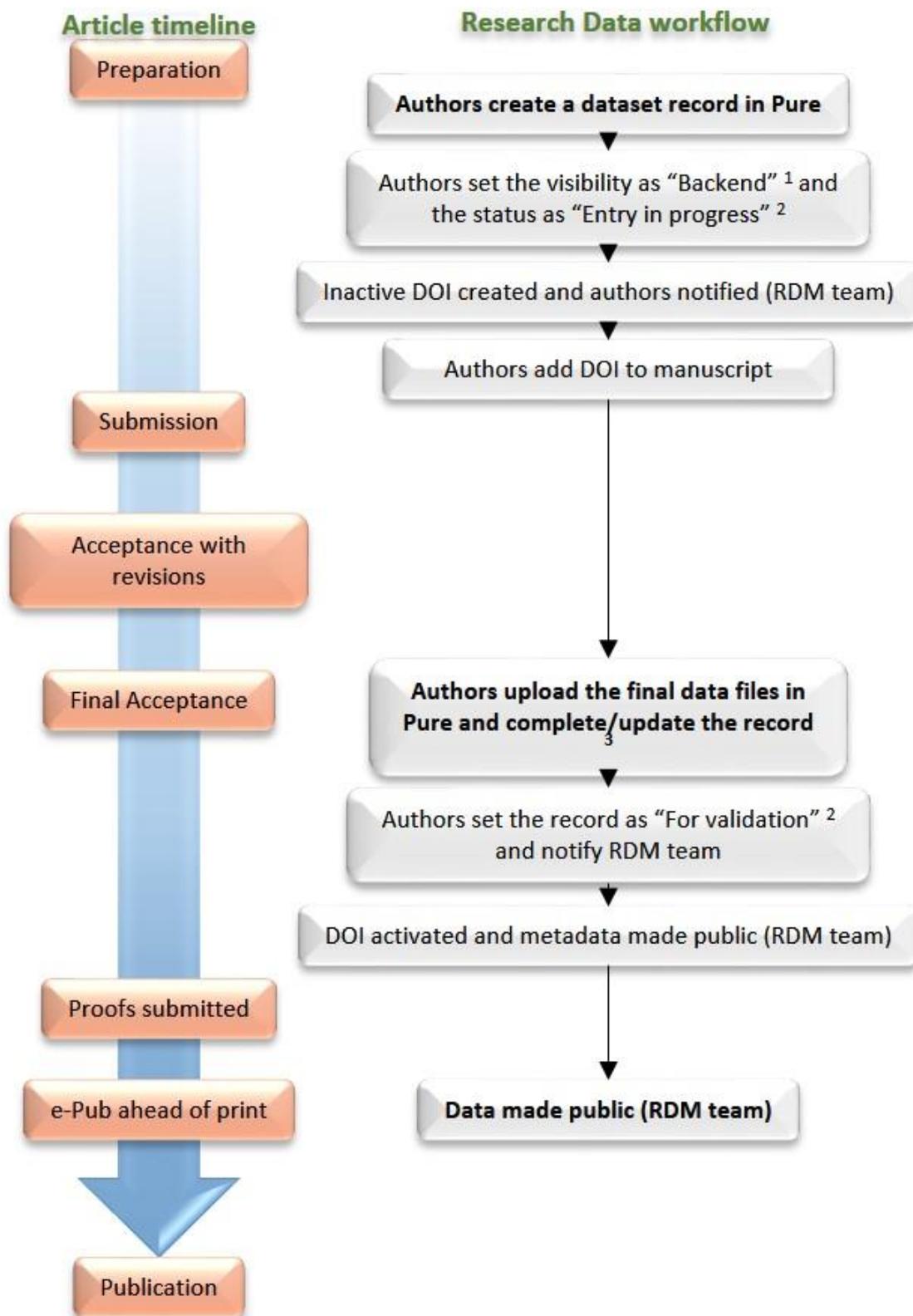
When you are about to submit your manuscript:

1. Create a basic dataset record in Pure:
 - Provide at least Title, Authors and Date made available (the year will be enough, The Library will fill in the rest of the date) (p. 5-7)
 - Set the metadata visibility as Backend – since the record is in preparation it should not be publicly visible yet (p. 8)
 - Set the status as “Entry in progress” (p. 8)
 - let us know if you require your data to be made public straightaway, for example for access by the referees
2. We will email you an INACTIVE DOI
3. Add the DOI to the manuscript using:

“The research data (and/or materials) supporting this publication can be accessed at [DOI]”
4. Submit your manuscript

After your manuscript has been accepted and is ready for publication:

5. Upload your final data files in Pure (for more details on file visibility see p. 8), check that title, authors and year made available are correct and set the status as “For Validation” (p. 9). IMPORTANT: until we validate the record the files will not be visible by the public.
6. Send us an email asking to activate the DOI and to let us know when and on what terms the data should be published. Please note that for this step the metadata (title, authors, description and publisher) will be made publicly available on the [University’s portal](#). It is important you notify us if for some reason this cannot happen (ex.: Journal policy).
7. Once the article is published we will validate the record. If you have set an embargo date on your datasets (p. 7-8) they will not appear on the portal until the embargo expires.



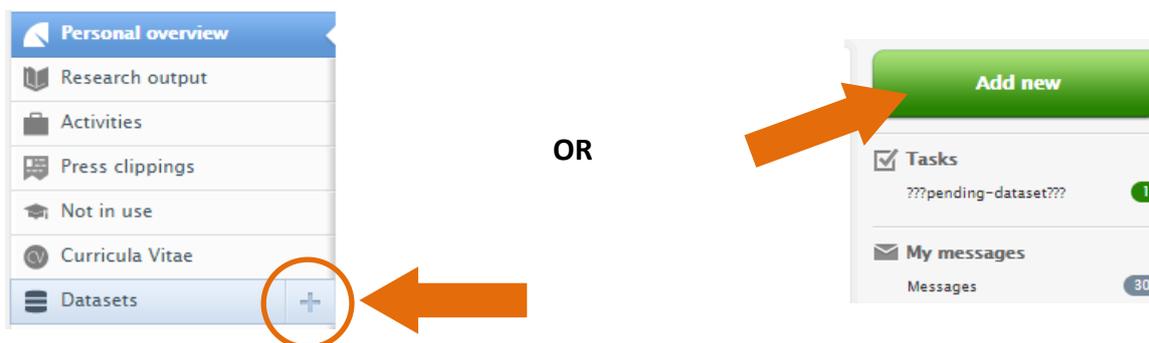
¹User Guide: "Depositing datasets in Pure: when and how", p.5

²User Guide: "Depositing datasets in Pure: when and how", p.5

³Check the title, add/update the dataset description, link to the publication and the projects in Pure (User Guide p.5 – Relation to content)

How to deposit

Log in into Pure at <https://www.st-andrews.ac.uk/staff/research/pure/>. From your personal profile you can open a Datasets template by clicking on **Add New** (on the right-hand side of the screen) and selecting **Datasets** from the **Choose submission** window; or by clicking on the '+' beside 'Datasets' on the left-hand side menu



Identification

Title: We advise to use the form: "Data underpinning – *Title of the article*".

Description: you should briefly describe the dataset, what type of files are attached and in which formats, if proprietary software is required (provide details) and any other relevant information that can help the user understand the datasets. More detailed information could also be provided as a ReadMe.txt file alongside the data files. See appendix for more details and examples.

Identification ?

Title *

Description

Temporal coverage

Year Month Day – Year Month Day

Date of data production

Specific date

Period of time

Temporal coverage: it indicates the date range coverage of the data, for example data covers animal records from 1850-1905.

Date of data production: this can either be a specific date or a period of time over which the data have been collected/produced. Please note that this field becomes mandatory only if one of the two options is selected.

Date of data production

Specific date

Year * Month Day

Period of time

Year * Month Day – Year Month Day

–

People

This will be pre-populated with your details. You would need to add the remaining authors as they appear on the paper. You can add either internal or external authors by clicking on “Add person...”.

Search for authors that are internal to the University

Create an author from a different institution or organisation

Search and add Person - or create External Person

Affiliation on the dataset

Managing organisational unit

This sections will be pre-populated with your details. It can be changed to a co-author’s internal organisational unit (School) if deemed more appropriate.

Data availability

Publisher: this is set by default to “University of St Andrews”. You should leave it as default unless you are creating a record for data deposited in another repository (e.g.: the data were deposited by a co-author in another university’s repository).

DOI: if a DOI does not exist the Library will provide you with one and fill in this field. If the data are published in another repository or database and a DOI already exists you can “Add existing DOI”.

Electronic data: this is where the files can be uploaded. After having selected the file, the ‘Multiple file upload’ window will open.

Data availability ⓘ

Publisher *
 University of St Andrews
 Publisher

DOI
 -or- If you do not have a DOI already one will be issued during validation where appropriate

Electronic data

Drag files or **browse** your computer.
 Max filesize: 1024 MB.

Physical data

Links

Date made available
 Year * Month Day

Multiple file upload						
File name	File size	Visibility	License	Type	Embargoed until	
Test_file_2.docx	11 KB	Public - No restriction ▼	CC BY ▼	Audiovisual ▼	<input type="text"/>	
Test_file_1.docx	11 KB	Public - No restriction ▼	CC BY ▼	Audiovisual ▼	<input type="text"/>	

Visibility – this can be either Public (after validation the files will be visible on the portal) or Backend (after validation the files will **not** show on the portal). Even if set as “Public” we will wait for the publication of the article before publishing the data. Please contact us if you are not sure what to set.

Depositing datasets in Pure: when and how

License – Please, choose a licence as this will inform the user on the terms and conditions of use. You can either use Creative Commons or Open Data Commons licences. For more information contact us or visit <http://creativecommons.org/> and <http://opendatacommons.org/>.

Type – make sure that the appropriate type is selected.

Embargoed until – you can decide when the files will become visible on the portal.

Physical data: here you can describe any physical item that can be made available upon request (e.g.: samples, tissues, notebooks, etc.).

Date made available: you can simply add the year and we will fill in the rest when the files will become publicly available.

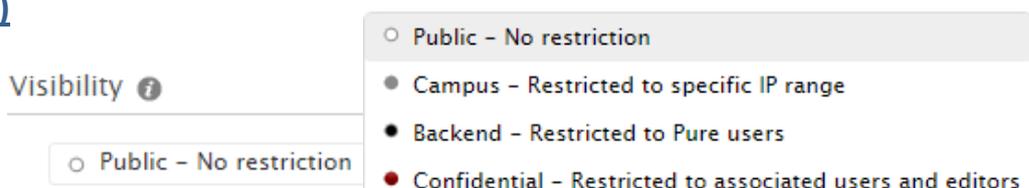
Access option - For Library use only

Relation to content

In this section you will be able to make links to other items in Pure. As a minimum you should link to the relative article and the grants associated with it. You can create a link by clicking on the “+” icon and searching by Title, Pure ID or Grant number. If you need any assistance, please get in touch.

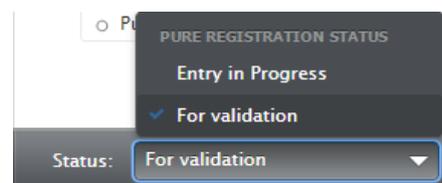
Visibility (metadata)

This will dictate if the metadata (general information: Title, description, authors, publisher, etc.) will be publicly visible on the University’s portal. **IMPORTANT:** This will be set as public for the activation of the DOI.



Status

By default this is set as “For validation”, you should change it to “Entry in progress” for as long as the record is not complete. Once the files have been uploaded and you require the activation of the DOI, please, set it as “For validation”.



Save

Remember to save when done
or all the changes will be lost



University Advice and Guidance

University RDM website	https://www.st-andrews.ac.uk/library/services/researchsupport/researchdata/
Contact us	Email - research-data@st-andrews.ac.uk ; Phone – 01334 462343
Data upload Video Tutorial	http://researchdata.wp.st-andrews.ac.uk/ready-to-publish/
Licences	http://creativecommons.org/ ; http://opendatacommons.org/
Pure	https://www.st-andrews.ac.uk/staff/research/pure/
Research Portal	https://risweb.st-andrews.ac.uk/portal/
General Pure enquiries	Pure Live System - purelive@st-andrews.ac.uk

Appendix

With your data you should provide enough information to give some context. This can take the form of a simple description (in the “Description” field), a more comprehensive ReadMe.txt file or both. You should include basic information on the methodology employed to acquire the data (online surveys, paper surveys, instrumental analyses, etc.) together with type of files, their formats and what software is required to open, visualise and analyse them. If you have any questions or would like some help, please do not hesitate to get in touch.

Example of Description:

The attached data files underpin the publication “*The title of your article*”. The following file types and formats are included:

- X-ray photoelectron spectroscopy files: .vms (can be opened with a text editor)
- X-ray diffraction files: .xrdml (proprietary format) and .udf (can be opened with a text editor)
- UV-Vis spectroscopy files: .jws (proprietary format) and .txt (can be opened with a text editor)
- Transmission electron microscopy: .dm3 (proprietary format) and .jpg

More details on the software required are provided in the ReadMe.txt file.

Example of ReadMe.txt file

The X-ray Photoelectron Spectroscopy (XPS) data have been acquired using a Kratos AXIS Ultra DLD, with a monochromatic Al Ka (1486.6 eV) X-ray source. The files are in .vms format and can be opened with any text file handling software (Notepad, Word etc.). The proprietary software that would allow for the visualisation of the data and their analysis is CasaXPS (<http://www.casaxps.com/>).

The powder X-ray diffraction data were collected using an Empyrean PANalytical series 2 diffractometer with a Cu Ka radiation source ($\lambda = 1.5406 \text{ \AA}$). The files are offered in two different formats:

- .xrdml, an xml coding that can be opened with the Notepad application and with the PANalytical software;
- .udf, that can be opened with any text handling software. It contains details of the analysis and the intensity counts.

To perform analysis on this data files software such as PANalytical may be required.

The UV-Vis spectra were acquired using JASCO-V-650 spectrophotometer. The files are in both proprietary file (.jws) and text file (.txt). The proprietary format requires the software SpectraManager by JASCO to be opened this software will also allow to perform further analysis of the data.

Transmission electron microscopy images were acquired using a Jeol JEM-2011 operated at 200 KV using a Gatan 794 CCD camera to record digital images. The original images are in .dm3 format which can be visualised with the free software ImageJ but require the Gatan software to be analysed. Images in .jpeg format have also been included.