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21 Feb 2018

Mendeley Data Evaluation Partnership

Supporting data management and sharing

Rosie Higman
Research Data Librarian
The University of Manchester Library

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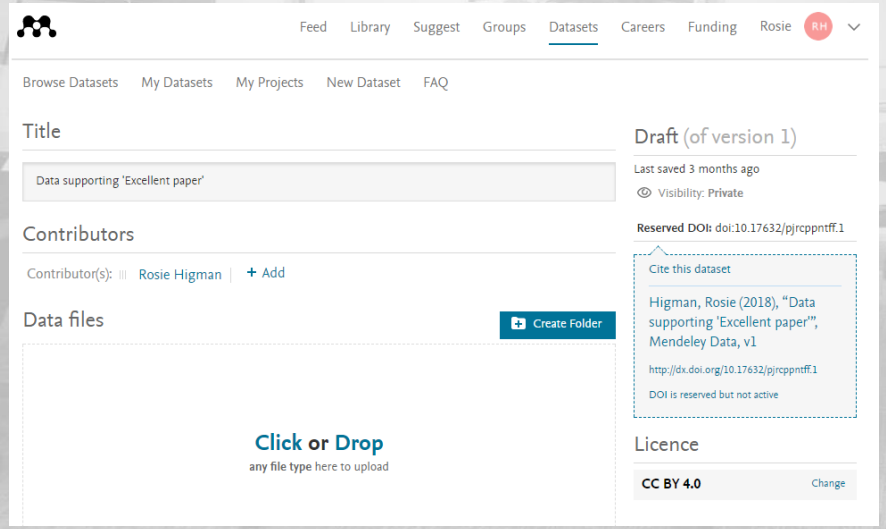
WHAT?

Two year project evaluating Mendeley Data platforms, including the data repository and manager, as part of the Research Lifecycle Programme.



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WHY?

Collecting metadata throughout the research process will make it easier to share results and data at the point of publication.

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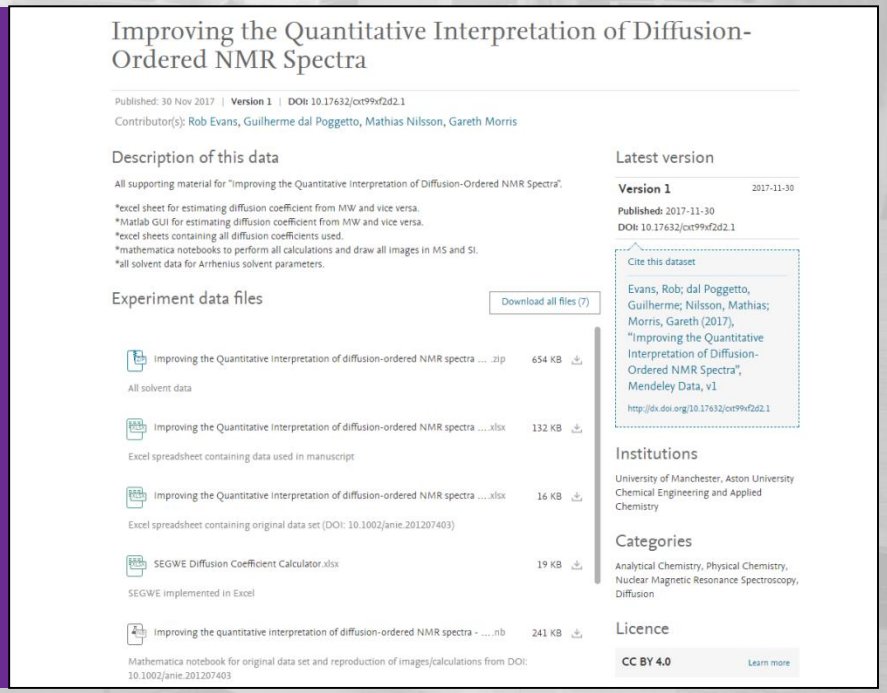
HOW CAN MENDELEY HELP YOU?

REPOSITORY

Visibility

Citations and impact

Journal and funder compliance



Improving the Quantitative Interpretation of Diffusion-Ordered NMR Spectra

Published: 30 Nov 2017 | **Version 1** | **DOI:** 10.17632/cxt99xf2d2.1

Contributor(s): Rob Evans, Guilherme dal Poggetto, Mathias Nilsson, Gareth Morris

Description of this data

All supporting material for "Improving the Quantitative Interpretation of Diffusion-Ordered NMR Spectra".

*excel sheet for estimating diffusion coefficient from MW and vice versa.
*Matlab GUI for estimating diffusion coefficient from MW and vice versa.
*excel sheets containing all diffusion coefficients used.
*mathematica notebooks to perform all calculations and draw all images in MS and SI.
*all solvent data for Arrhenius solvent parameters.

Experiment data files

Download all files (7)

Improving the Quantitative Interpretation of diffusion-ordered NMR spectra .... .zip 654 KB
All solvent data

Improving the Quantitative Interpretation of diffusion-ordered NMR spectra ....xlsx 132 KB
Excel spreadsheet containing data used in manuscript

Improving the Quantitative Interpretation of diffusion-ordered NMR spectra ....xlsx 16 KB
Excel spreadsheet containing original data set (DOI: 10.1002/anie.201207403)

SEGWE Diffusion Coefficient Calculator.xlsx 19 KB
SEGWE implemented in Excel

Improving the quantitative interpretation of diffusion-ordered NMR spectra - ....nb 241 KB
Mathematica notebook for original data set and reproduction of images/calculations from DOI: 10.1002/anie.201207403

Latest version

Version 1 2017-11-30

Published: 2017-11-30
DOI: 10.17632/cxt99xf2d2.1

Cite this dataset

Evans, Rob; dal Poggetto, Guilherme; Nilsson, Mathias; Morris, Gareth (2017), "Improving the Quantitative Interpretation of Diffusion-Ordered NMR Spectra", Mendeley Data, v1
http://dx.doi.org/10.17632/cxt99xf2d2.1

Institutions

University of Manchester, Aston University
Chemical Engineering and Applied Chemistry

Categories

Analytical Chemistry, Physical Chemistry, Nuclear Magnetic Resonance Spectroscopy, Diffusion

Licence

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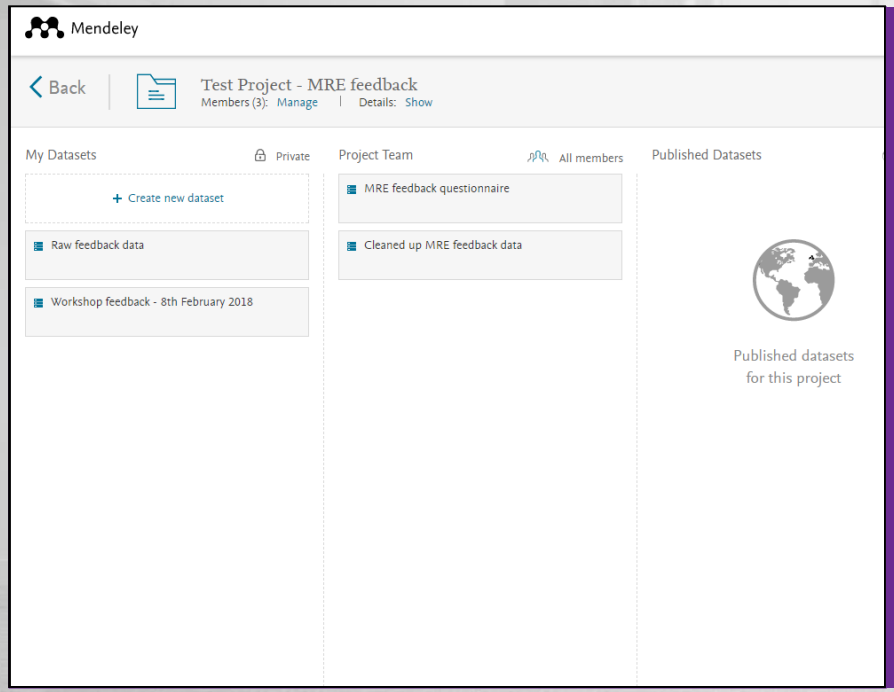
HOW CAN MENDELEY HELP YOU?



MANAGER

Saving time

Improving data quality

Enabling collaboration

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DEVELOPMENT PLANS

Recent changes

- Folders
- Upgrade to 100GB per dataset allowance
- First version of Data Manager
- Basic showcase

Coming soon

- File tagging
- CAS authentication
- Custom metadata
- File referencing with Dropbox
- Working towards Isilon integration

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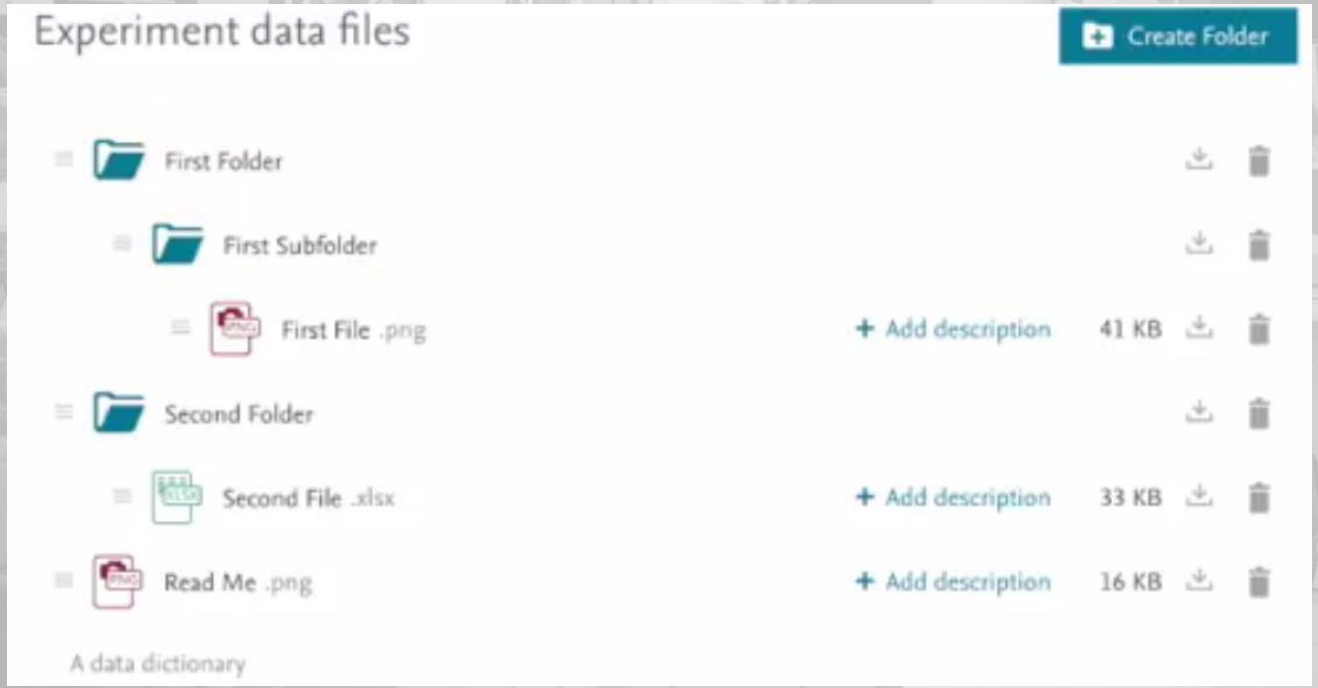
FOLDERS



Demo: https://www.youtube.com/watch?v=FpO3l2C-8LA

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SHOWCASE

University of Manchester

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Discover curated datasets from the University of Manchester

ZIP

FESTA: an efficient NMR approach for the structural analysis of mixtures containing fluorinated species

Gareth Morris, Pinelopi Moutzouri, Thaís Mendonça Barbosa, Cláudio Tormena, Roberto Rittner, Andrew Phillips, Steven Coombes, Laura Castañar, Mathias Nilsson

13 Feb 2018 in: Nuclear Magnetic Resonance Spectroscopy

Bruker pulse sequences and experimental data for FESTA methods for the analysis of mixtures of 19F-containing species by measurement of doubly selective 1D TCOSY 1H spectra

CSV

(De-)Stabilising effects of a transition

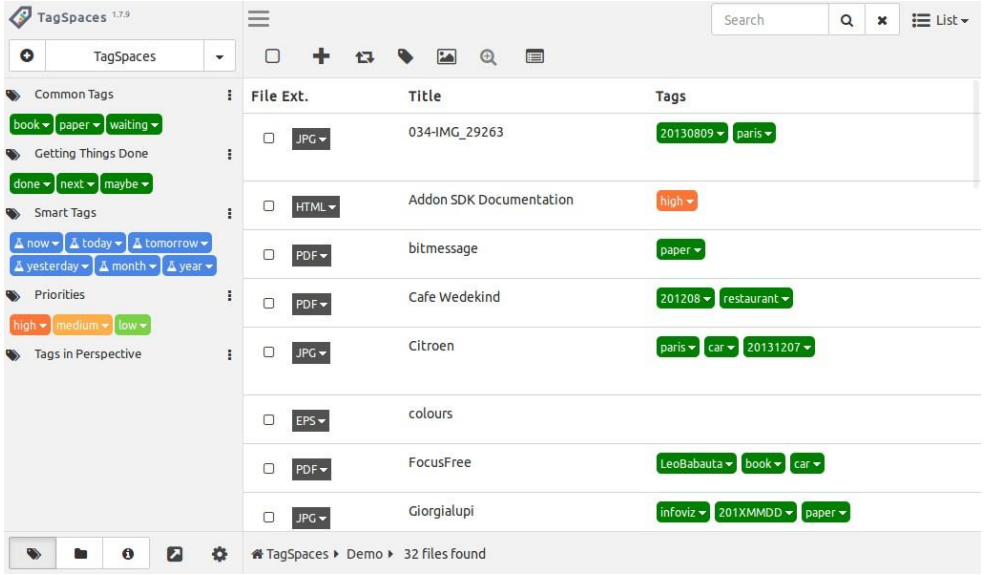
Julia Kasmire

02 Feb 2018 in: Agent-Based Modeling, Diffusion of Innovation, Transitions

This data set is the raw output of an experiment testing how stability can be measured over time in relation to a simulated transition

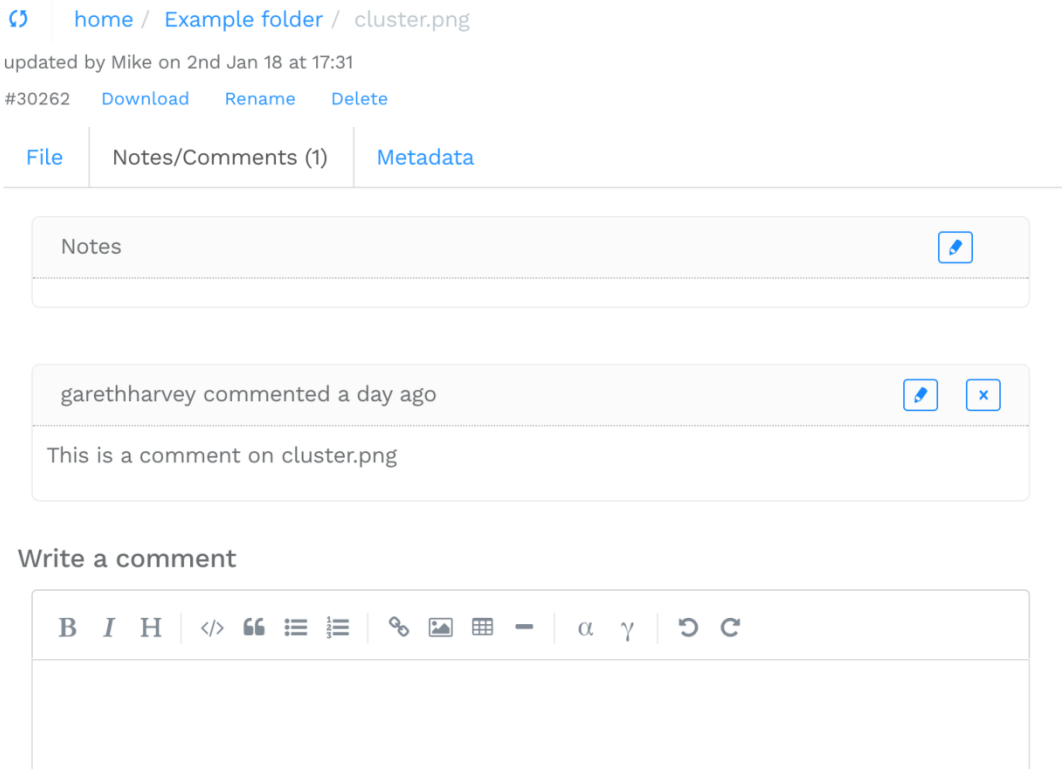
File Tagging

- Free text tags allowing researchers to quickly and simply annotate files
- Provides quick and simple way to find files
- Can be aggregated up to the dataset level (i.e. add all of the tags to the dataset)
- Previously entered tags for a project are suggested as future tags for consistency (within the project)



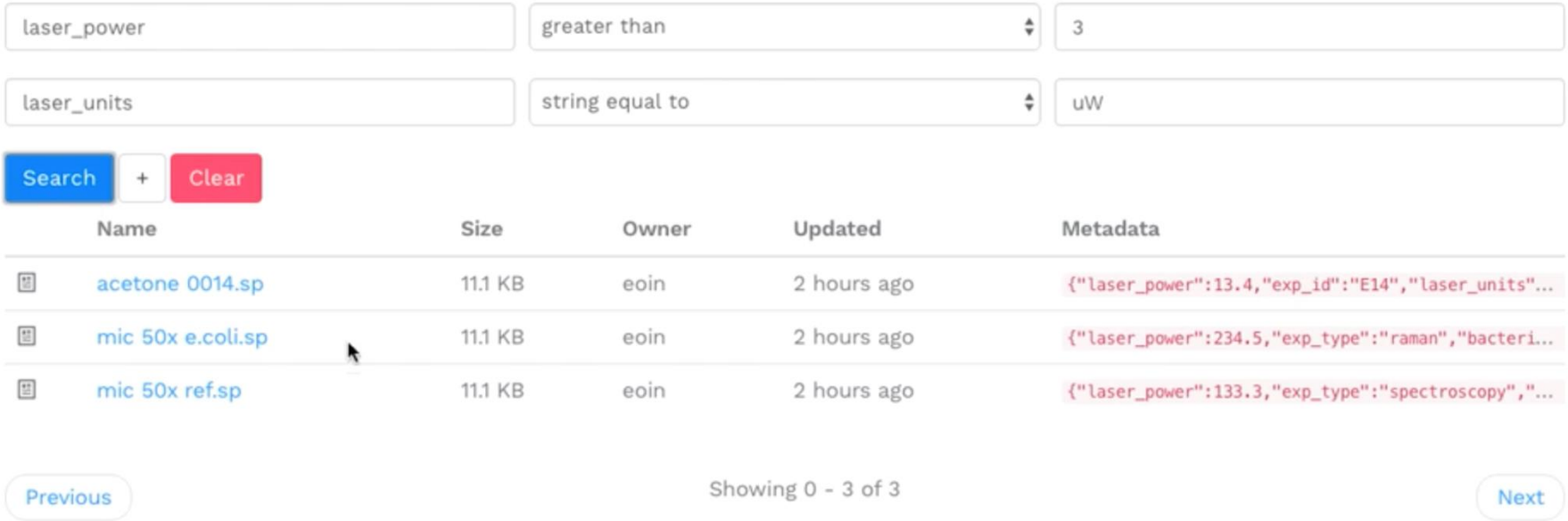
File Commenting

- Allow comments against each file
- Comments include reference to the person who made the comment and the date/time the comment was made
- Optionally can send a notification to the owner of the file, or other people who have commented previously
- Comments are private by default and are not shown on published datasets, but are available for review by project members and approvers in draft datasets



File Custom Metadata

1. Allow researchers to **add custom metadata** (i.e. key-value pairs) to files
2. Allow researchers to **find files** using this metadata (e.g. see below from https://rinocloud.com/)
3. Allow researchers to **aggregate** custom metadata at the **Dataset level** (if required)
4. **Automatically** add any metadata for an **experiment** (e.g. researcher, date completed, experiment title etc.) to any associated file
5. Allow researchers to create **metadata templates**, and associate to file types (e.g. all BAM files use the “Gene” template)
6. **Automatically add metadata** where technically feasible e.g. extract from file (e.g. NetCDF) or inherit from containing folder (e.g. watch folder for Spectrometer XYZ).



Folder Types

Internal Folder (Mendeley Data)

- Files are stored within Mendeley Data's S3 file store.
- Files and folders can be uploaded, as with Datasets

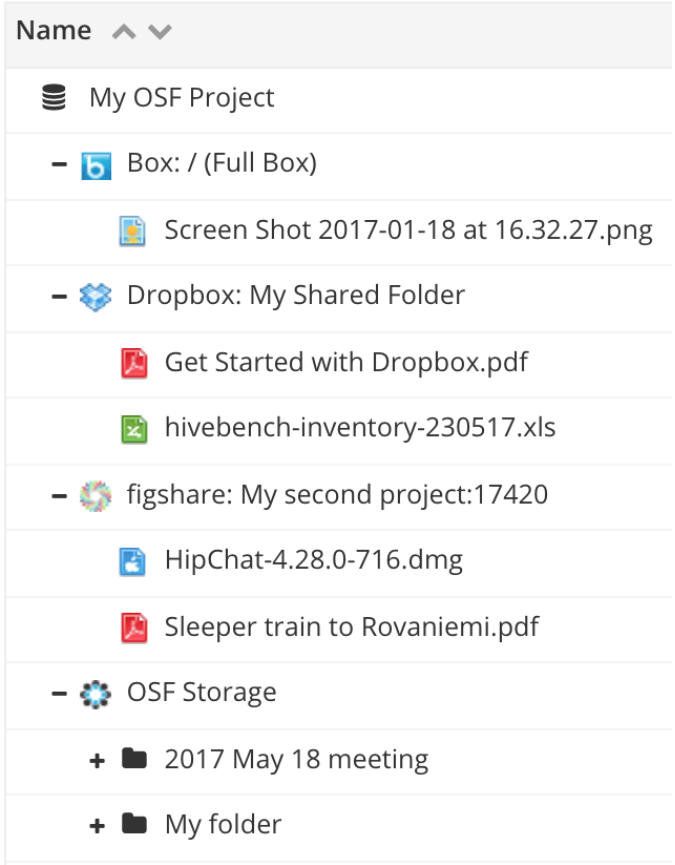
External Folder (Referenced)

- Files are stored within an external file storage platform (e.g. DropBox, Box, Google Drive etc.)
- Clear visual distinction made between local folders (& files) and external folders (& files) e.g. see OSF approach on right
- File contents of these folders can change

Watch Folder

- Watch folder is a type of external folder where researcher can be notified when files have been added or changed
- This could happen within the application (see example below) or via optional email notification

File	Added	Last Modified
12345.csv	12 Jan 2018	12 Jan 2018
6789.csv	18 Jan 2018	**20 Jan 2018***
abcdef.csv*	**20 Jan 2018**	**20 Jan 2018**



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HOW CAN YOU GET INVOLVED?

Join the RDAG	Find out about new features first, regular discussions, email list for updates, Sifter for issue logging
Try it out	If you have data to share try using Mendeley Data and then…
Send us feedback!	We want to hear the good, the bad and the suggestions for improvement at researchdata@manchester.ac.uk