

A guide to uploading files to the Imperial HPC Data Repository

1. Set yourself up with an ORCID identification (if you do not already have one) at orcid.org.
2. Sign into the Data Repository (data.hpc.imperial.ac.uk), first through your Imperial ID and then through ORCID. In the top left hand corner of the page you will see the following list of options:

Browse
Add Collection
Deposit Data
Persistent URL
Tools
Github Integration
Help

3. Each new set of data (i.e. all the data you want to upload for a publication) is called a collection. To start a new dataset, click 'Add Collection'.
4. Name your collection and add a description (you must have something in the description category). Tip: paper title and abstract work well for the title and description, respectively. Click 'submit'.

Browse	<h2>Create Collection</h2> <table border="1"><thead><tr><th>Description</th><th>File</th></tr></thead><tbody><tr><td>Title</td><td>Paper title</td></tr><tr><td></td><td>Abstract</td></tr><tr><td>Description</td><td></td></tr></tbody></table> <p>Member of <input type="text"/></p> <p><input type="button" value="Submit"/></p>	Description	File	Title	Paper title		Abstract	Description	
Description		File							
Title		Paper title							
		Abstract							
Description									
Add Collection									
Deposit Data									
Persistent URL									
Tools									
Github Integration									
Help									

5. Once you have clicked submit, a DOI is generated for the data. The DOI is private and is embargoed. Any external person wishing to view any data under this DOI will either need the access code or you will need to release the embargo.

Browse
Add Collection
Deposit Data
Persistent URL
Tools
Github Integration
Help

Publication Successful

The DOI of your deposition is [10.14469/hpc/2084](https://doi.org/10.14469/hpc/2084)

- To obtain the access code or release the embargo, go to 'Browse' and select the collection.

Browse	<h1>Paper title</h1> <p>DOI: 10.14469/hpc/2084 Metadata</p> <p>Created: 2017-01-18 11:52</p> <p>Author: Clare Bakewell</p> <p>Abstract</p> <h2>Embargo</h2> <p>Access code: f9dy-knnt</p> <p>Release embargo</p> <p>Edit</p>
Add Collection	
Deposit Data	
Persistent URL	
Tools	
Github Integration	
Help	

- To add data to your collection click 'Deposit Data'. Choose the file(s) you would like to upload, add a title and a description. Uploading each file individually is advised (click 'add file' to choose another file another) and once the files are uploaded select the data to be a 'Member of' the relevant collection. Click 'submit'. A DOI for the data deposition is created.

Browse	<h1>Deposit Data</h1> <h2>Select files to upload</h2> <table border="1"><thead><tr><th>Description</th><th>File</th></tr></thead><tbody><tr><td>Title</td><td>Example upload</td></tr><tr><td>Description</td><td>Word document </td></tr></tbody></table> <p>File 1 <input type="button" value="Choose Files"/> <input type="button" value="Example upload"/> <input type="text" value="Word doc."/></p> <p><input type="button" value="Add file"/> <input type="button" value="Delete selected"/></p> <p>Member of <input type="text" value="Paper title -- 10.14469/hpc/2084"/></p> <p><input type="button" value="Submit"/></p>	Description	File	Title	Example upload	Description	Word document
Description		File					
Title		Example upload					
Description		Word document					
Add Collection							
Deposit Data							
Persistent URL							
Tools							
Github Integration							
Help							

If you now browse your collection, the data is listed; in this case as 'Example upload', clicking on the DOI allows access to the uploaded files associated with 'Example upload'. It is useful to create new data depositions for each set of data you upload (for instance data type or experiment/compound names).

Screen
Add Collection
Deposit Data
Permalink URL
Tools
Upload Information
Help

Paper title

DOI: [10.14469/hpc/2084 Metadata](#)

Created: 2017-01-18 11:52

Last modified: 2017-01-18 12:24

Author: [Clare Bakewell](#)

Abstract

Embargo

Access code: P9dy-knnt

[Release embargo](#)

Members

DOI	Description
10.14469/hpc/2095	Example upload

[Edit](#)

8. Clicking on 'edit' allows you to modify your collection. Here you can add any associated DOIs to your collection, and list both internal and external collaborators.
9. Once all of your files are uploaded you're ready to go. Share the DOI with anyone you want to share the data with. Don't forget to either provide them with the access code or release the embargo.

Note: It is not possible to delete data once uploaded. However, if you make a mistake you can redirect your data to a different collection. We suggest making a reject collection, any unwanted uploads can be made a 'member of' the reject collection.

A guide to uploading NMR data (MestReNova & mnpub):

When uploading MestReNova files, the data repository will automatically generate a **.mnpub** file. The file can be viewed with unlicensed versions of MestReNova, meaning the data can be viewed even if you don't use the same software or access to the software licence, therefore truly open access.

1. You will need MestReNova 11.
2. Create one MestReNova file per compound. Create a separate Chemdraw file with the associated compound structure (Chemdraw files need to be saved as .cdxml in order to generate metadata).
3. Deposit data in a 'collection' as described above. Upload the files individually i.e. the MestReNova file as 'file 1' and the Chemdraw file as 'file 2'. Any other data associated with the compound may also be uploaded.
4. When you upload the MestReNova and Chemdraw files, a **.mnpub** file will automatically be generated. In addition to this, Metadata is generated.

Files

Filename	Size	Type	Description
Compound2b.cdxml	8KB	chemical/x-cdxml	Compound 2b Chemdraw file
Compound2b.mnova	2MB	chemical/x-mnova	Compound 2b Mnova file
Compound2b.mnpub	0	chemical/x-mnpub	Mestrenova signature file for Compound2b.mnova

Member of

DOI	Description
10.14469/hpc/1726	Addition of Carbon-Fluorine Bonds to a Mg(I)-Mg(I) bond: An Equivalent of Grignard Formation in Solution

Metadata

Key	Value
inchi	InChI=1S/C6F5.C5H10Ar2N2.Mg/c7-2-1-3(8)5(10)6(11)4(2)9;1-4(8-6)3-5(2)9-7;/h;4-5H,3H2,1-2H3;/q;-2;+2
inchikey	MUZAOUHLJFPKAY-UHFFFAOYSA-N
inchikey	Usage: babel [-i<input-type>] <name> [-o<output-type>] <name>

[Edit](#)

5. The mnpub files generated will not be able to be viewed until the embargo has been removed. i.e. when the data is made public.