

Organising & standardising research data that underpin your publication

Willeke de Haan, KU Leuven Research Coordination Office

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Overview

- Organise and structure data and documentation files linked to a publication during and after research
- Logical, structured and descriptive file names
- Open / standard file formats
- File versioning in a project
- Data standards to make data interoperable, commonly understandable and reusable (the I and R of FAIR)



Organise / structure files

- Different options exist
- Here examples of good practices that researchers at KU Leuven use
- Find what works for you, in line with technical knowledge / support available and your data collection methods and active data storage system
- Centre organisation around:
 - Research project
 - Research paper



Folder structure

- File Explorer, OneDrive, MS Teams, ...
- Develop a structure organised by:
 - Paper, Project, Researcher, Experiment, Instrument
- Folders should:
 - follow a structure with folders and subfolders that correspond to the project design and workflow
 - have a self-explanatory name that is only as long as is necessary
 - have a unique name
- Consider read / write access to folders for colleagues / collaborators
- Good practice: ReadMe file in top folder
- When paper is published (or end of project): package structure and files into zip bundle and move to archival storage

An example: project/ code/ code needed to go from input files to final results raw and primary data (never edit!) data/ raw external/ raw internal/ meta/ documentation of the study doc/ intermediate/ output files from intermediate analysis steps logs/ logs from the different analysis steps notebooks/ notebooks that document your day-to-day work results/ output from workflows and analyses figures/ reports/ tables/ temporary files that can safely be deleted or lost scratch/ README.txt file and folder description

Source: https://rdmkit.elixir-europe.org/data organisation

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Example

ProjectName

README file that lists the folder structure explaining the content of each folder, incl date of last update

- •Data: Separate folder for all fixed raw data used in the project that do not change throughout the project
 - •Subfolders for individual datasets + information file explaining methods used and relevant parameters to create the data
- •Preprocessing:
 - •Subfolders for each step in preprocessing, in chronological order with date at start of subfolder name (track sequence of analytical steps)
 - •Within each **subfolder** ReadMe file with links to relevant wiki pages, source code files
 - •Within each **subfolder** scripts developed and resulting intermediate data together: script describes how this version of data was processed from the previous version.
- •Analysis:
 - •Subfolders for each experiment, in chronological order by using the date at the start of a subfolder name
 - Scripts
 - Outputs
 - Results
- •Sourcecode: self-developed code or models + ReadMe file with link to git repository
 - •Active: sandbow for active development of code where best practices are not expected
 - •Release: final version of code
- •Doc: documentation files for the project, incl papers
- •Datapoints: folder for intermediate datasets for use in future; if during preprocessing / analysis you obtain a useful intermediate dataset you may use in future, copy it here to a subfolder, with relevant script; include ReadMe file to explain how datapoint was created
- •Temp: Folder for draft versions of data and codes you want to keep. Move them here from "Analysis" if no longer relevant there



Record file

- A textual or tabular record file can list all data and documentation files of a project, paper, etc. This can record standard information for each dataset:
 - Unique ID
 - Dataset name
 - Description
 - Origin
 - Owner
 - Person responsible
 - Purpose, e.g. project name
 - Storage location, e.g. where on server, OneDrive, etc.
 - Contains personal data Y/N
 - Size / volume
 - Access: who has / needs access to the data

Within our research group we mostly develop algorithms for simulations. Every researcher has to keep a register in the form of a Word file that lists which code repositories (on GitLab or GitHub) are used (URL) and where data files are stored. These registers are available on a sub-website and colleagues have read access.



eLab Notebook

- eLab notebook systems (e.g. LabCollector, eLabFTW) can be used as registry to note and point to or include data files, protocols, experiments, documentation, samples used, etc.
- Some allow files to be uploaded into the notebook or file paths can be used
- When paper is published: export overview of all experiments, descriptions and links to data files to single PDF file as documentation
- End of a project: export all data, annexes and documents to zip files for archiving

A lab uses eLabFTW as electronic lab notebook. Researchers use tablets in the lab to record their experiments. They use templates for different experiments and included databases, cell lines, reference data and protocols that are frequently used within the lab, so researchers can simply point to those. Researchers can set up 'to do' lists at the start of their experiment, and sign those off as they proceed. Each PhD researcher has to use the electronic lab book to record all steps in his/her experiment, upload or point to protocols, import data files, etc. Supervisors have read access, can include comments and use the lab notebook for PhD progress discussions. When a PhD project ends, the lab exports a zip file (bundle) of the entire lab notebook of that person for archiving. This contains the lab book as single PDF file, with all annexes organised in folders.



Data management plan

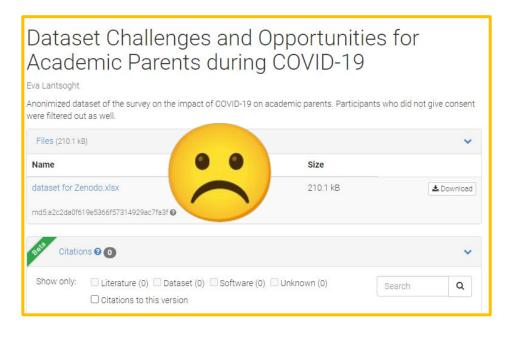
- Records all data files generated and used for a researcher project / paper
- Describes how data are used / generated, who is responsible, where data are held (stored), etc.
- Details all accompanying documentation files and any relevant ethical, legal or compliance details

In our research group we work with existing third party datasets that we acquire. Before a dataset is imported for use, a data management plan has to be written by the researcher that provides information on what the dataset will be used for, where it was obtained, who needs to have access to the dataset, which licence conditions apply, etc.



File naming

- Develop a logical structure for meaningful file names
- Order 4-7 elements from generic to specific
- Suggested elements:
 - Project / experiment name, acronym or number
 - Creator name or initials
 - Date of creation: use ISO8601 format YYYYMMDD (and if needed time HHMMSS)
 - Type of data: sample ID
 - Version number: v01, v02, 00.01, 01.01 (leading zeros ensure correct sorting of files)
 - Location
- No spaces: use underscore (_), hyphen (-) or Capitalized letters to separate elements
- Avoid special characters such as "/\: *?" <>[] & \$
- Independent of the location of the file on a computer
- Include a txt-file that explains your naming convention in your documentation





File naming examples

Honeybee project, experiment 2 done in Helsinki, data file created on the second of December 2020

- File name: 20201202_HB_EXP2_HEL_DATA_V03.xls
- Explanation:
 Date_ProjectAbbreviation_ExperimentNumber_Location_TypeOfData_VersionNumber

Cropped image of an ant head taken on the third of December 2020 by Meg Megson

- File name: 20201203_MM_HEAD_CROPPED_V1.psd
- Explanation: Date_CreatorData_Type_Modification_Version

Version 4 of the survey procedures for the British Dental Health Survey.

- BDHS_SurveyProcedures_00-04.pdf
- Explanation: Project acronym_Type_version number

Source: https://rdmkit.elixir-europe.org/data_organisation

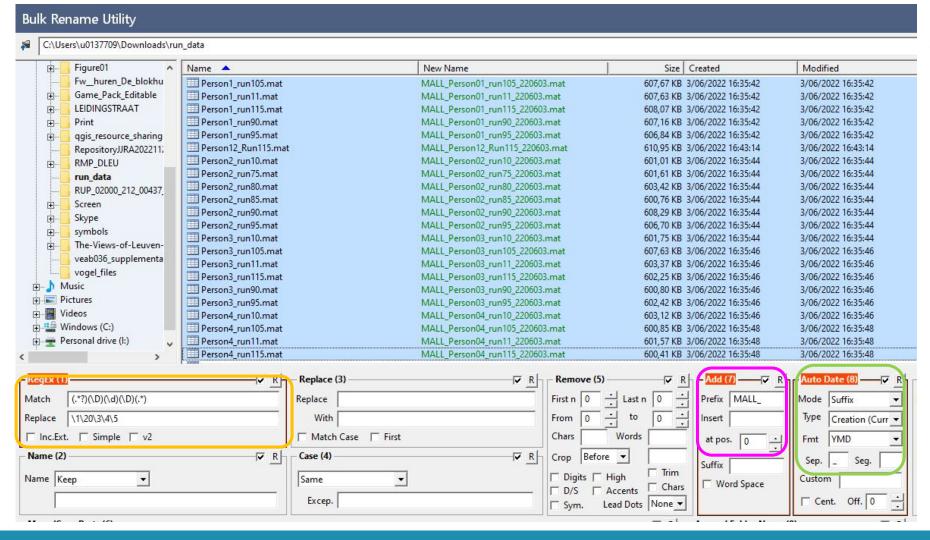


Batch file renaming

- Need to rename large amounts of file names?
 - Images from digital cameras with automatically assigned files names/numbers
 - Default filenames generated by proprietary software or instruments
 - Removing spaces, odd characters, etc
 - Add meaningful elements to file name, e.g. project acronym, date, etc.
- Use a batch renaming tool for consistent, structured renaming
 - Bulk Rename Utility (Windows)
 - Renamer (Mac)
 - Gnome Commander (Linux)
- Demo: Renaming Files Using Bulk Rename Utility YouTube



Batch rename example



Experiment measuring vertical dynamic running load with 13 treadmill users.

File renaming for 78 files:

- Find single digits in filename and add leading zero
- Add project name 'MALL' as prefix
- Add creation date as suffix, with underscore

Exercise: folder structure & file naming

- The role of basial epithelial cells for small airway loss and epithelial injury in chronic lung disease.
 - Design a suitable folder structure for this research project
 - What would be useful elements for file names?



Exercise: folder structure & file naming

Folders

- Data
 - Scans
 - Processed data
 - Images
 - Measures
- Doc
 - SOP
 - ...
 - Papers
- Code
- Results

Elements

- Whole, Part
- Lung
- Sample number
- Collection date
- Donor pseudoniem
- Replication number
- Control, COPD, IPF
- Mild, moderate, severe



Open / standard file formats

- Use or convert to open / standard file formats when you can
- For long-term access and use of research data
- Good source: fairsharing.org
 - Images: TIFF, JPEG 2000, PNG, GIF
 - Text: XML, PDF/A, HTML, JSON, TXT, RTF
 - · Containers: TAR, ZIP
 - Databases: XML, CSV, JSON
 - Video: MPEG (mp4), AVI
 - Sounds: WAVE, AIFF, MP3, FLAC
 - Statistics: DTA, POR, SAS, SAV
 - Tabular data: CSV, TXT
 - 3D: X3D, C3D
 - Microscopy: <u>OME Next Generation File Format</u>, Bio-formats conversions
 - Neuroimaging: <u>DICOM</u>, <u>Nifti</u>
 - Mass spectrometry: <u>mzML</u>
 - Sequencing data: <u>FASTA</u>, <u>FASTQ</u>



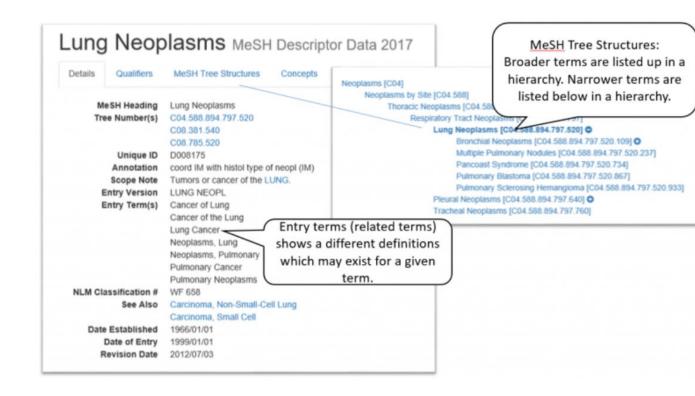
File versioning

- Manage multiple versions of the same file / document
- Enable reverting to an earlier version
- Easy methods for small demands of versioning:
 - File naming
 - Version control log in file
 - Cloud storage service with automatic file versioning, e.g. OneDrive
- For automatic management of versioning, conflict resolution and back-tracing capabilities, use a proper version control software such as Git, e.g. GitHub, GitLab, BitBucket: next presentation this afternoon



Data standards

- Use data standards to make data interoperable, easier to understand (by multiple communities) and reusable more widely
 - International, common standards
 - Community standards



Standards

International

- ISO 8601 standards for date / time
- ISO 3166 standard for country codes
- Getty Thesaurus for geographical names

Community

- DICOM MRI data
- NACE code: Statistical classification of economic activities in European Community
- Standard International Age Classification, UNStat 1982

- C. Learning and education services
 - Enrolment in regular and adult education
 - 2. Educational attainment
 - 3. Illiteracy
- Health, health services and nutrition
 - Morbitiy and handicaps (for mortality see I)
 - 2. Usage of health services
 - 3. Food consumption
 - 4. Malnutrition
- D. Earning activities and the inactive
 - 1. Labour force participation
 - Employment/unemployment/ underemployment

```
| 2-4; 5 y.gr. 5-24; 10 y.gr. 25-64; 65+
| 5 y.gr. 15-24; 10 y.gr. 25-64; 65+
| 5 y.gr. 10-24; 10 y.gr. 25-64; 65+
```





PollEv.com/willekedehaan890



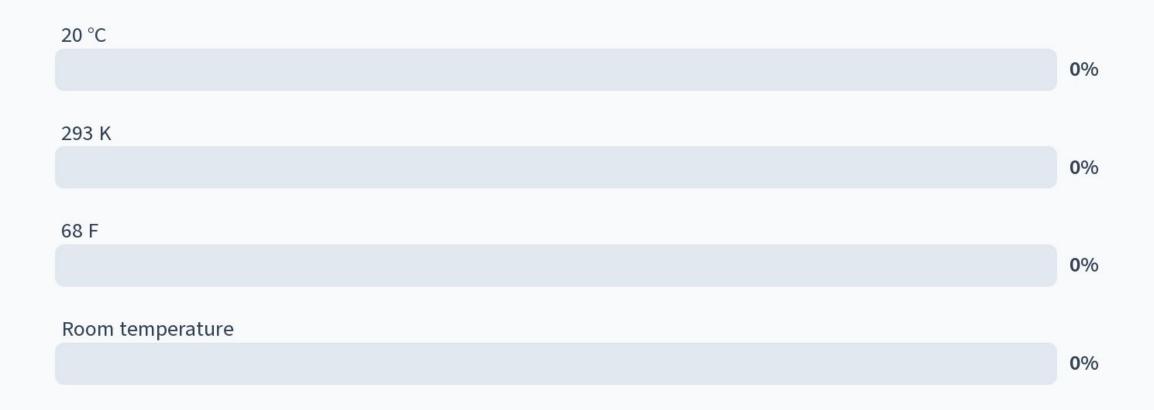
To aks participants about their history of using tobacco, which is probably not a value in the Common Data Element (CDE) "Smoke History Status"?

Never smoked	
	0%
Former smoker	
	0%
Current smoker	
	0%
Heavy smoker	
	0%
Unknown	
	0%

Which is a unique identifier for aspirine?

DB00945 (Drugbank online)	
	0%
CHEBI:15365 (Chemical Entities of Biological Interest dictionary)	
	0%
CO1405 (KEGG Compound Database)	
	0%
Acetylsalicylic acid	
	0%





Which answer options are suitable to ask about how much participants exercise

not; once in a while; sometimes; often; all the time 0% <1 hour; 1-2 hours; 2-4 hours; >4 hours per week 0% hours per week 0% 0% light exercise, moderate exercise, vigorous exercise 0%

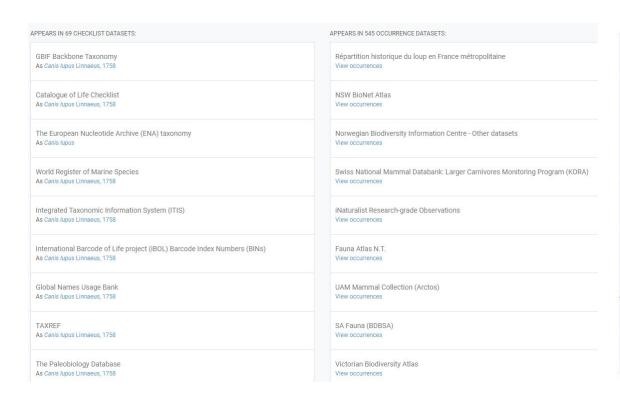


Nobody has responded yet.

Hang tight! Responses are coming in.

GBIF & Darwin Core

Appears in Datasets



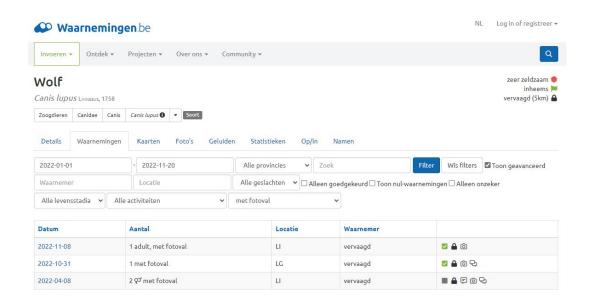
Darwin Core standard

Record-level Terms	Dublin Core terms, institutions, collections, nature of data record	
Occurrence	evidence of species in nature, observers, behavior, associated media, references.	
Event	sampling protocols and methods, date, time, field notes	
Location	geography, locality descriptions, spatial data	Simple Darwin Core (flat)
Identification	linkage between Taxon and Occurrence	
Taxon	scientific names, vernacular names, names usages, taxon concepts, and the relationships between them	
GeologicalContext	geologic time, chrono-stratigraphy, biostratigraphy, lithostratigraphy	
ResourceRelationship	explicit relationships between identified resources (e.g., one organism to another, taxon to location, etc.)	Generic Darwin
MeasurementOrFact	measurements, facts, characteristics, assertions, references	Core (relational)



Community standard: biodiversity data

Wolf observations Flanders 2022



Because biodiversity data are collected worldwide using the same data standards, collecting the same attributes and variables, they can be combined into large comparable datasets on the GBIF platform.

GBIF platform wolf data 2022

Canis lupus Linnaeus, 1758 Arctic Wolf In English Basionym: Lupus lupus Linnaeus, 1758 OVERVIEW 4 TREATMENTS METRICS REFERENCE TAXON = 9.740 OCCURRENCES WITH IMAGES EXPLORE = 7 0 %

Compatible dates: Linking 5 minute weather data with time of sunrise / sunset

TimeStamp in both datasets facilitates interoperability

													77	-010000	-	0000		20.50	
d	A	В	C	D	E	F	G	Н	1	1	K	L	8	20180306	6	0804	1908	11.07	S
1	TimeStamp	Time	Td	Tw	RH	Sdur		Sdur_accum_der	TSoil5	TSoil10	TSoil20	TSoil30	0						ccum_de
1	UTC	hhmm	degC	degC	%	sec		h	degC	degC	degC	degC	9	20180307	/	0801	1910	11.13	
3	20180308	0005	4.78	4.14	93.5	0	0.00	0.00	5.64	5.77	5.84	5.87	10	20180308	8	0759	1912	11.22	0
4	20180308	0010	4.84	4.15	92.8	0	0.00	0.00	5.63	5.76	5.84	5.87	11	20180309	9	0756	1914	11.28	0
5	20180308	0015	4.83	4.08	92.0	0	0.00	0.00	5.63	5.75	5.83	5.87							0
6	20180308	0020	4.86	4.06	91.2	0	0.00	0.00	5.62	5.74	5.82	5.86	12	20180310	U	0754	1916	11.37	0
7	20180308	0025	4.72	3.95	90.8	0	0.00	0.00	5.62	5.73	5.81	5.87	13	20180311	1	0751	1918	11.43	0
8	20180308	0030	4.53	3.77	90.1	0	0.00	0.00	5.62	5.73	5.81	5.86	14	20180312	2	0749	1920	11.52	0
9	20180308	0035	4.52	3.74	90.1	0	0.00	0.00	5.62	5.72	5.80	5.86			-				0
10	20180308	0040	4.50	3.71	90.4	0	0.00	0.00	5.61	5.72	5.79	5.86	15	20180313	3	0746	1922	11.58	0
11	20180308	0045	4.51	3.71	90.4	0	0.00	0.00	5.61	5.71	5.79	5.86	16	20180314	4	0744	1924	11.67	0
12	20180308	0050	4.49	3.69	90.2	0	0.00	0.00	5.61	5.70	5.78	5.86	17	2018031	5	07/11	1926	11 72	0
13	20180308	0055	4.49	3.67	90.0	0	0.00	0.00	5.62	5.70	5.77	5.85	5.35	5.77	-0.1		0.0		0
14	20180308	0100	4.48	3.67	90.2	0	0.00	0.00	5.61	5.70	5.77	5.85	5.35	5.77	-0.2		0.0	0.0	0
		24.00																	

В

hhmm

0816

0814

0811

0809

0806

2 UTC

20180301

20180302

20180303

20180304

20180305

TimeStamp Sunrise Sunset DayLer gth

hhmm hrs

1858

1900

1902

1904

1906

10.70

10.77

10.83

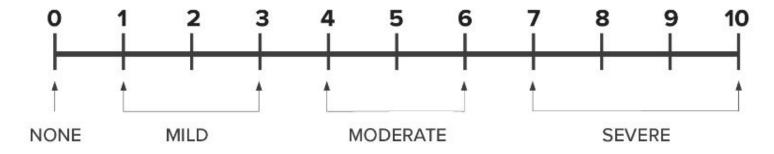
10.92

10.98

NIH Common Data Elements

0 - 10 Numeric Pain Rating Scale

Element (CDE) is a standardized, precisely defined question, paired with a set of allowable responses, used systematically across different sites, studies, or clinical trials to ensure consistent data collection.



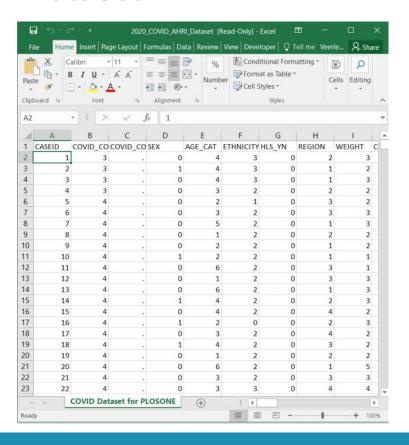
Categorical Scale





Codebook to understand data

Dataset



Codebook

1	A	В	
1	VAR	Description	Response Options (if applicable)
2	CASEID	Case ID	
3	COVID_COHORTS_4	Cohorts (4): Pos, Neg, Untested, Not suspected	1:Positive; 2:Negative; 3:Untested; 4:COVID Not-Suspected
4	COVID_COHORTS_2	Cohorst (2): Pos, Neg	1:Positive; 2:Negative
5	SEX	Sex	0:Female; 1:Male
6	AGE_CAT	Age categorized	1:18-24 years; 2:25-34 years; 3:35-44 years; 4:45-54 years; 5:5
7	ETHNICITY	Ethnicity	0:Other or more than 1; 1:Black or African American; 2:White;
8	HLS_YN	Hispanic, Latino, or Spanish origin	0:No; 1:Yes
9	REGION	Region	1:Northwest; 2:Midwest; 3:South; 4:West
10	WEIGHT	Weight categorized (self-reported)	1:Under weight; 2:Normal weight; 3:Slightly overweight; 4:Mod
11	CCI_SCORE	Charlson Comorbidity Score	
12	CCI_HBP	Hypertension	0:No; 1:Yes
13	CCI_DB_NO_COMPL	Diabetes (Type I or Type II) without complication	0:No; 1:Yes
14	CCI_COPD_BR_EMP	Chronic lung disease (COPD), chronic bronchitis	0:No; 1:Yes
15	CCI_HA	Heart attack	0:No; 1:Yes
16	CCI_CHF	Congestive heart failure	0:No; 1:Yes
17	CCI_STROKE_TIA	Stroke or transient ischemic attack (TIA)	0:No; 1:Yes
18	CCI_LV_MILD	Mild liver disease, hepatitis, cirrhosis	0:No; 1:Yes
19	CCI_DB_COMPL	Diabetes (Type I or Type II) with chronic compli	0:No; 1:Yes
20	CCI_PVD	Peripheral vascular disease	0:No; 1:Yes
21	CCI_LV_MOD_SEV	Moderate or severe liver disease, hepatitis, cirr	0:No; 1:Yes
22	CARE_PHY_YN	Physician visit or call (telemedicine)	0:No; 1:Yes
23	CARE_ER_YN	Emergency room visit	0:No; 1:Yes
24	CARE_HOSP_YN	Hospital visit (stay of one or more nights)	0:No; 1:Yes
25	AB_RESULT	Antibody test result positive or negative	0:Negative; 1:Positive; 2:Not sure
26	SYM_FEVER	Fever	0:No; 1:Yes
27	SYM_COUGH	Dry cough	0:No; 1:Yes



Lego replication game



Lego replication game: discussion

- Structured templates help to write out instructions
 - Standardises the process
- Brick lists help to write out instructions
 - Reduces ambiguity

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- Standardises naming
- Brick lists could have unique numbers / codes for each brick
- = controlled vocabulary / community standard
- Visuals help: drawing or pictures of vehicel



Research Coordination Office

Standardisation ...



6x2 brick



flag



4x2 brick



4x2 brick with slope



3x2 brick



2x2 brick with slope



2x2 brick



3x2 brick with slope



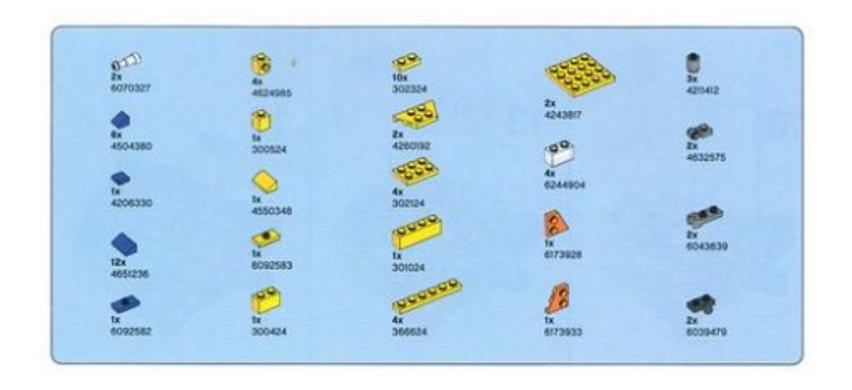
4x1 brick



tall 2x1 brick with slope

DETAILED	INSTRUCTIONS	
Step	Parts required	Instructions
1		
2		

· ·			
DETAIL	ED INSTRUCTIONS	S	
Step	Part shape	Part colour	Instructions
1			
2	10.		
3	8.		6.



Take away messages

- When you start a project, design your folder structure and file naming system
- When you end your project / publish your paper, check your folder structure / file names are still in order (or fix), then zip and archive your data
- Use open / standard file formats when you can to make your data FAIR
- Use data standards where you can, to make your data interoperable and FAIR