Various and voluminous data

Master of Applied IT – Semester 2

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Context

This research aims to explore and document various file types generated by experiments in the fields of Supramolecular and Inorganic chemistry, particularly focusing on data generated by the RobotLab project (research words obtained from use cases of RobotLab documentation). The primary objective is assessing the compatibility of NOMAD Oasis on the various and voluminous data. NOMAD Oasis is a local instance of the central NOMAD infrastructure and is a data management platform.

Data from different sources are gathered to compile a comprehensive list of various file types, with their file size. This includes files from partner universities' experiments and supplementary research publications.

Key objectives of the research include:

- **Identification of Data Formats**
  Determine the various data formats generated by experiments.
- **Identification of Data Volume**
  Estimated volume of data generated by the RobotLab project's experiments.
- **Evaluation of NOMAD Oasis Compatibility**
  Assess the support for various and voluminous data types expected from the RobotLab project. This evaluation will help determine the suitability of NOMAD Oasis as a data management solution for the RobotLab project.

Through this research, we aim to address the following questions:

- What data formats will be generated by the RobotLab project? (E.g., videos, images, formulas)
- How much data is anticipated to be generated on a regular basis by the RobotLab project?
- Is the support for standard data formats in NOMAD Oasis relevant to the diverse data types expected from the RobotLab project?

By providing a comprehensive analysis of file types and assessing the compatibility of NOMAD Oasis, this research will contribute to the research of finding a suitable data management platform for the RobotLab project.

Used instruments

Radboud University created a list of different analysis types with the used equipment.

Nr	Analysis type	Equipment type	Person in charge	Src
1	**Automation platform**	ChemSpeeds	Wilhelm	
2	**Peptide synthesizer**	Biotage Syro II	Wojtek	1
3	**Peptide purification**	Biotage Extrahera	Wojtek	2
4	**DLS**	Wyatt DynaPro Plate Reader	Mathijs	3
5	**Liquid handling robotics**	OpenTrons OT-2 (P20, P1000)	Will	4
6	**Liquid handling robotics**	OpenTrons OT-2 (P20, P300) + Heater Shaker Module	Will	5
7	**pH meter**	Hudson Rapid pH	Mathijs	6
8	**Rheometer/viscometer**	Unchained Labs Honeybun	Mathijs	7
9	**DLS/SLS/UV**	Unchained Labs Stunner	Mathijs	8
10	**DLS/SLS/Fluorescence**	Unchaned Labs Uncle	Mathijs	9
11	**Flow induced dispersion analysis (FIDA)**	FidaBio	Evan	10
12	**Viscosity**	Rheosense VROC Initium	Wojtek	11
13	**Liquid dispenser**	Dispendix i.DOT	Wilhelm	12
14	**Nefelometer**	NEPHELOstar Plus	Wilhelm/Mathijs	13
15	**Online Infrared measurement**	ReactIR	Will	14
16	**Chromatography**	HPLC	-	-
17	Deep Learning Workstation	Computer	Will/Stefan	-

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[3] https://www.wyatt.com/products/instruments/dynapro-dynamic-light-scattering-plate-reader.html

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[9] https://www.unchainedlabs.com/uncle/

[10] https://www.fidabio.com/product

[11] https://www.rheosense.com/products/viscometers/vroc-initium-one-plus

[12] https://dispendix.com/idot-non-contact-liquid-handler

[13] https://www.bmglabtech.com/en/nephelostar-plus/

[14] https://www.mt.com/gb/en/home/products/L1_AutochemProducts/ftir-and-raman-spectrometers/ftir-spectrometers.html

18	Absorbance/fluorescence/luminescence in multi-well plates	Tecan Spark plate reader	Wojtek	15
19	Zetasizer	Zetasizer APS	Mathijs	16

Table 1: Instruments

File types

In this paragraph, file types are gathered to help researching various and voluminous data generated by experiments, and testing these on the NOMAD Oasis instance

Each file type is documented in a table, with some information of that file that helps determining the contents and importance of the file.

File type	Contents	Category	Size	Total size
File extension	Description on contents of the file.	File category (Described below)	File size	Total size of all files with specific type.

Table 2: File type table layout

File category:

- **Text Files**
  These are often used for raw data output from various instruments. They can contain numerical data, metadata about the experiment, or even results from computations.
- **Comma-Separated Values**
  This format is commonly used for tabular data.
- **Video's**
  Video's can be generated from many experiments like microscopy.
- **Images**
  Images can be generated from a variety of sources, such as microscopy or spectroscopy data. They can also be used to visually represent certain types of data.
- **Spectra Files**
  These files are used to store spectral data from techniques like NMR, IR, UV-Vis, FTIR etc.
- **Tabular**
  Tabular files are commonly used to organize and analyze large amounts of data.
- **Chemical Structure Files**
  These files are used to represent the 3D structures of molecules. They can be generated by software used for molecular modeling or crystallography.
- **Collection Folder**
  This folder can contain multiple raw data files.

[15] https://lifesciences.tecan.com/multimode-plate-reader
[16] https://www.malvernpanalytical.com/en/support/product-support/zetasizer-range/zetasizer-aps

Unfortunately, there is a lack of available information regarding the raw files produced by the instruments. After discussions with both my company mentor and colleague, it has been determined that the manufacturers of these instruments are unwilling to disclose such details. Access to the output files is only granted after the delivery of the instrument.

Fortunately, we currently possess a few operational instruments that are generating data. With the assistance of TU/e and Radboud University, we have compiled the following list of their raw data types:

Radboud University

File type	Contents	Category	Size	Total size	Nomad support
.xls	Raw data from plate reader. For now, only analytical instrument being used beside camera.	Tabular data	87KB	-	✓
.json	Log file from OpenTrons, logging steps taken.	Text file	383KB	-	✓
.py	Procedure file of OpenTrons	Text file	1MB	-	✓

Table 3: Radboud University Raw data

Currently, Radboud University works with eLabFTW[17] which is a free and open source **E**lectronic **L**ab **N**otebook. eLabFTW is a system that tracks experiments efficiently, it is like a traditional notebook where scientists documented their experiments.

File type	Contents	Category	Size	Total size	Nomad support
.eln	Electronic Lab Notebook (eLabFTW) of example experiment.	Collection folder	37KB	37KB	✓

Table 4: Radboud University ELN

TU/e

File type	Contents	Category	Size	Total size	Nomad support
.ibw	-		16.MB		✓
.tri	-		317KB		✓
.001	-	Collection folder	983KB		✓

Table 5: TU/e Raw data

[17] https://www.elabftw.net/

Supplementary data

In addition to the raw data files from partner universities, supplementary data from published research is gathered to provide a more comprehensive list of data file types.

1. Confocal interferometric scattering microscopy reveals 3D nanoscopic structure and dynamics in live cells [1]

   Searched for: Microscopy

   Instrument: Confocal Laser Scanning Microscope with sCMOS camera

File type	Contents	Category	Size	Total size	Nomad support
.mp4	Fluorescence signal from mCherry-LaminA was recorded simultaneously. Images were background corrected to display the C-iSCAT contrast	Video	17MB	153MB	✓

Table 6: Supplementary Data

2. A general supramolecular strategy for fabricating full-color-tunable thermally activated delayed fluorescence materials [2]

   Searched for: Supramolecular

   Instrument: -

File type	Contents	Category	Size	Total size	Nomad support
.slsx	Table of Atomic coordinates	Chemical Structure Files	14KB	5MB	✓

Table 7: Supplementary Data

3. Scalable production of structurally colored composite films by shearing supramolecular composites of polymers and colloids [3]

   Searched for: Supramolecular

   Instrument: USB4000 fiber optical spectrometer (Ocean Optics)

File type	Contents	Category	Size	Total size	Nomad support
.xls	Reflectance at various wavelengths	Tabular data	20KB - 1MB	26MB	✓

Table 8: Supplementary Data

4. Silicon-RosIndolizine fluorophores with shortwave infrared absorption and emission profiles enable in vivo fluorescence imaging [4]
   Searched for: Fluorescence
   Instrument: Formulate nano emulsions for general systemic circulatorySWIR fluorescence imaging

File type	Contents	Category	Size	Total size	Nomad support
.xlsx	Molar absorptivity and normalized and corrected emission spectra in dichloromethane.	Tabular data	165KB	165KB	✓
.xlsx	Absorption spectra of fluorophores in the nanoemulsions, cross-sectional intensities from mouse imaging experiments, and capillary brightness.	Tabular data	150KB	150KB	✓
.xlsx	Capillary brightness data from depth penetration experiments.	Tabular data	221KB	221KB	✓

Table 9: Supplementary Data

5. Structurally diverse macrocycle co-crystals for solid-state luminescence modulation [5]
   Searched for: Luminescence
   Instrument: -

File type	Contents	Category	Size	Total size	Nomad support
.cif	Single-crystal structures	Chemical Structure Files	100kb-3MB	29MB	✓

Table 10: Supplementary Data

6. De novo determination of mosquitocidal Cry11Aa and Cry11Ba structures from naturally-occurring nanocrystals [6]
   Searched for: NEPHELOstar Plus && Nephelometer
   Instrument: MultiMode8

File type	Contents	Category	Size	Total size	Nomad support
.tar.gz	Gzipped Tarball file, collection of multiple files	Collection folder	44MB	44MB	✓
.spm	Setting/log file of MultiMode 8	Text file	6.4MB		✓

Table 11: Supplementary Data

7. Design of target specific peptide inhibitors using generative deep learning and molecular dynamics simulations [7]
   Searched for: Peptide Sequences
   Instrument: Simulation software data.

File type	Contents	Category	Size	Total size	Nomad support
.pdb	Protein Data Bank file, used to store 3d coordinates specifying the structure of atoms within a protein or other chemical compound.	Chemical structure file	333KB	1MB	✓
.xtc	Trajectory file format by GROMACS. File contains automic coordinates.	Text file	1.7MB	5.1MB	✓

Table 12: Supplementary Data

8. Crystallization of binary nanocrystal superlattices and the relevance of short-range attraction [8]
   Searched for: Crystallization
   Instrument: Software- HOOMD-Blue version 2.9.x

File type	Contents	Category	Size	Total size	Nomad support
.mp4	Time-dependent scattering pattern for the binary dispersion including larger *X* and smaller PbS nanocrystals at a stoichiometry of 1:2.	Video	333KB	1MB	✓
.py	Runs a simulation in which AlB2 is self-assembled inside	Text file	4.9KB	4.9KB	✓
.gsd	The initial configuration needed for the simulation	Text file	1.8MB	1.8MB	✓

Table 13: Supplementary Data

9. Creating nanoscale emulsions using condensation [9]
   Searched for: Emulsions
   Instrument: Nikon D-800 camera in video recording mode at 1920 x 1080 size and 30 fps

File type	Contents	Category	Size	Total size	Nomad support
.mov	Condensation of Water Droplets onto Dodecane	Video	8MB	16MB	✓

Table 14: Supplementary Data

10. Structural characterization and reactivity of a room-temperature-stable, antiaromatic cyclopentadienyl cation salt [10]
Searched for: Reactivity
Instrument: -

File type	Contents	Category	Size	Total size	Nomad support
.xyz	Files of all compounds calculated using different basis sets	Text file	3.8KB	95KB	✓
.txt	Files of calculated absolute energies, bonding energies, thermochemical data.	Text file	1.8KB	5.4KB	✓
.cif	Christallographic data	Chemical structure file	100kb-4MB	1MB-40MB	✓

Table 15: Supplementary Data

11. Scalable and continuous access to pure cyclic polymers enabled by 'quarantined' heterogeneous catalysts [11]
Searched for: Viscometry
Instrument: -

File type	Contents	Category	Size	Total size	Nomad support
.excl	CP-purity	Tabular data	164KB	164KB	✓
.excl	Temp dependence	Tabular data	10KB	10KB	✓
.excl	-	Tabular data	33KB	66KB	✓

Table 16: Supplementary Data

12. Auto-deconvolution and molecular networking of gas chromatography–mass spectrometry data [12]
Searched for: Gas chromatography
Instrument: -

File type	Contents	Category	Size	Total size	Nomad support
.excl	Deconvolution time testing data	Tabular data	26KB	26KB	✓
.excl	Global network cosine distribution data	Tabular data	3MB	3MB	✓

Table 17: Supplementary Data

13. Proton gradients and pH oscillations emerge from heat flow at the microscale

Searched for: pH-Measurement

Instrument: (vitrotubes 5003, CMScientific, UK) connected to a BTP E-60 tubing (0.76 × 1.22 mm, Instech Laboratories, Inc., USA) and a high precision syringe pump

File type	Contents	Category	Size	Total size	Nomad support
.avi	Formation of a stable pH gradient in a phosphate buffer solution.	Video	7.8MB	7.8MB	✓
.avi	Qualitative visualization of particle trajectories inside the flow chamber.	Video	8.4MB	8.4MB	✓

Table 18: Supplementary Data

NOMAD

Supported file types

All file types gathered in this research is supported by NOMAD. The data is not automatically parsed to understandable data for NOMAD.

NOMAD's documentation provides an overview of the various parsers available for different computational chemistry and physics software packages.[18] These parsers are designed to interpret and convert the output files fromexperiments into a standardized format that NOMAD can understand and process.

- **Parsers Overview**
  Parsers are crucial for enabling NOMAD to analyze data from a wide range of file formats.
- **Functionality**
  Parsers extract essential information such as calculation results, system configurations, and electronic structures from raw files.
- **Compatibility**
  The documentation lists parsers for many popular software packages, but also allows for customization of parsers.
- **Details**
  Each parser that is provided by NOMAD includes the format homepage, plugin name, parser class, and a link to the parser code.

For the data from this research, there is no parser that supports parsing of the raw data. However, as mentioned above, it is possible to create a custom parser that helps the support of data generated by the RobotLab project.

Supported file volume

NOMAD has specific limitations regarding the size and number of unpublished data uploads to maintain data manageability. These restrictions include[19]:

- Each upload must not exceed 32 GB in size.
- Users can have a maximum of 10 unpublished uploads within a NOMAD Oasis instance.
- Only uploads with at least one recognized entry are eligible for publishing.

The files researched in this context do not surpass NOMAD's upload limits. The largest experimental data includes videos of 16MB, totaling 153 MB in size. The maximum of 10 unpublished uploads, relates to publications within the Oasis, not to central NOMAD.

[18] https://nomad-lab.eu/prod/v1/staging/docs/reference/parsers.html#elabftw
[19] https://nomad-lab.eu/prod/v1/staging/docs/howto/manage/upload.html#upload-limits

GUI- Upload process raw files

NOMAD is based on a *bottom-up* approach to data management. Instead of only supporting data in a specific predefined format, files are processed to extract data from an extendable variety of data formats. Converting heterogenous files into homogeneous processed data is the basis to make data FAIR.

For this example, two files from Radboud University are used:

- **PDA004_03.xlsx**
  Raw data from plate reader. For now, only analytical instrument being used beside camera.
- **PDA004_03.json**
  Log file from OpenTrons, logging steps taken.

Step 1: Create a new upload.

A new upload can be created by adding raw files in the GUI. Files can be uploaded as ZIP or as separate files.

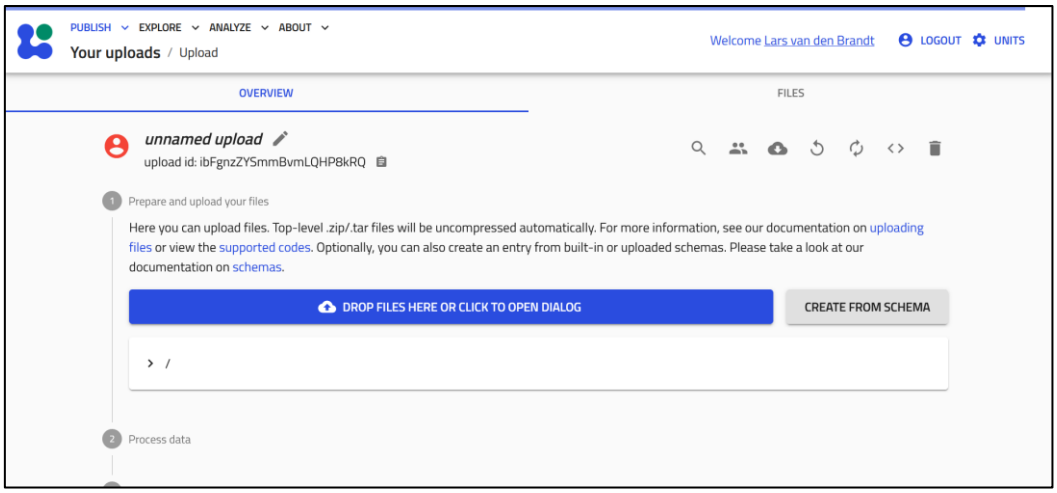

Figure 1: Create new upload

Step 2: Review file structure.

After files are uploaded, files can be viewed in folder structure as uploaded. The GUI gives the possibility to preview the uploaded file. Review all files and make sure there are no errors.

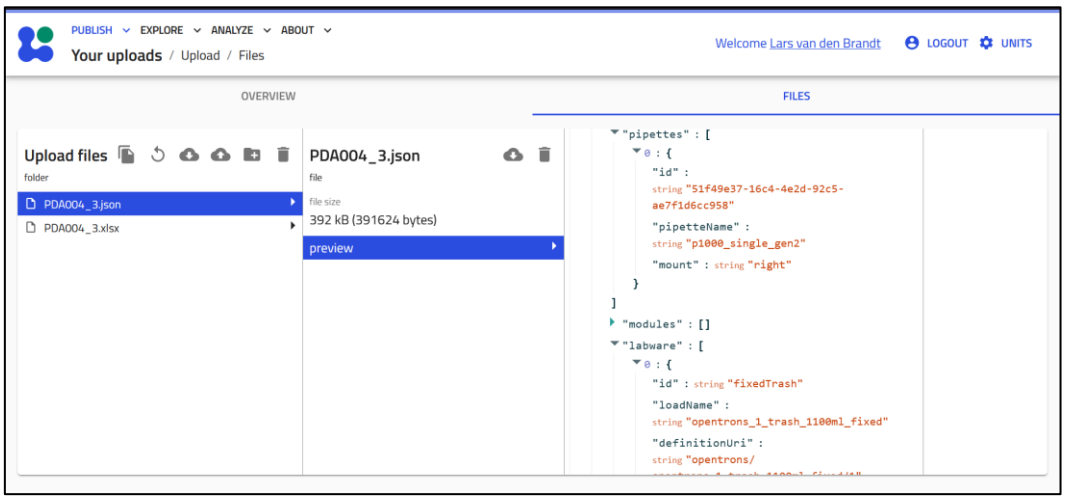

Figure 2: View file structure

Step 3: Select schema for parsing.

After all of entry are uploaded, a schema can be selected for parsing. First name the entry, then select either a built-in schema, or select a custom schema.

For this example, the Basic ELN built-in schema is selected. Custom schema's will be researched with another sub-question.

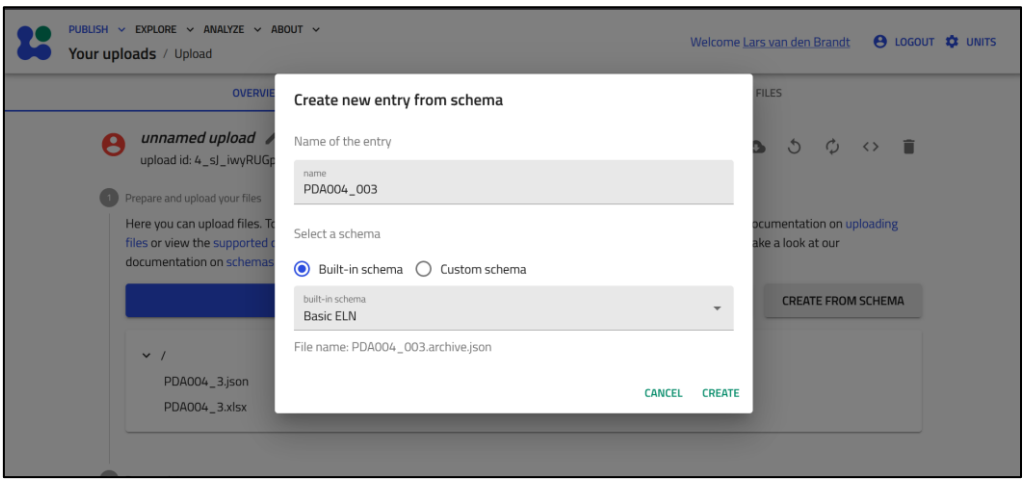

Figure 3: Select schema

Step 4: View data & add data

After the files are parsed, the heterogeneous files should have been parsed to understandable readable data. Unfortunately, there is no available parser for the .xlsx file generated from the plate reader.

By selecting the Basic ELN (in step 3), a template is created where a description with tags is displayed. In my example, there was no data because there was no available parser, I added the data manually.

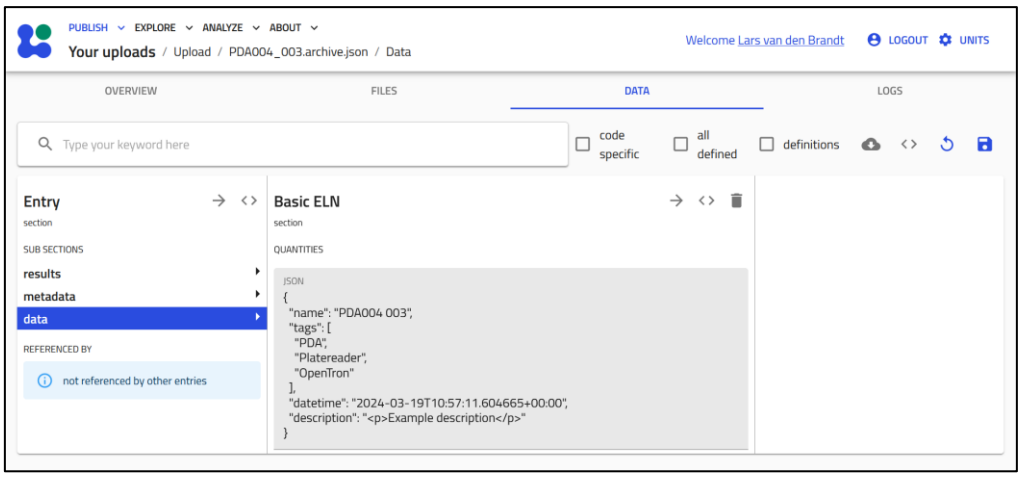

Figure 4: View & add data

Step 5: Edit author metadata

You can add more information about your data, like *comments (co-authors)*, *references* (e.g. links to publications).

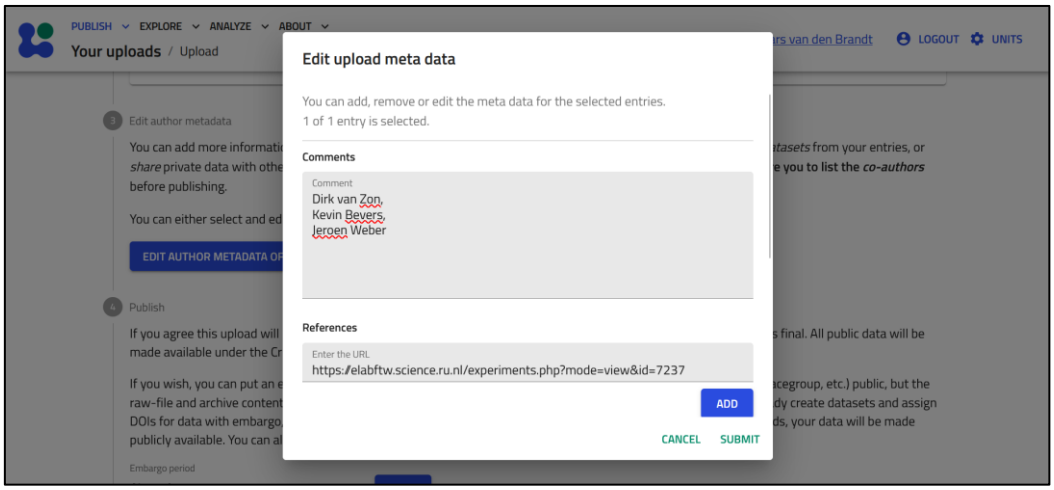

Figure 5: Add author metadata

Step 6: Publish to NOMAD Oasis

Finally, publish the upload directly to the NOMAD Oasis, or publish with an embargo up to 36 months.

After uploading to NOMAD Oasis, there is an option to publish to NOMAD central.

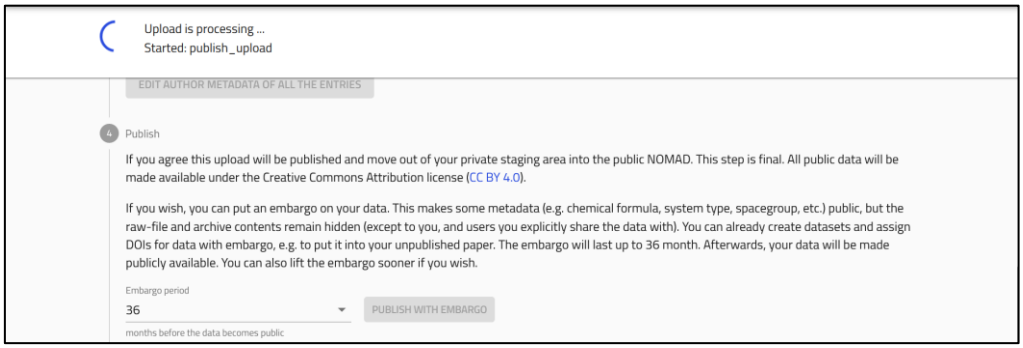

Figure 6: Add author metadata

CMD – Upload process eLabFTW

NOMAD offers all its functionality through **A**pplication **P**rogramming **I**nterfaces (API's). Specifically RESTful HTTP API's. This allows us to us NOMAD as a set of resources that can be uploaded, accessed, downloaded, and searched through HTTP requests.

For this example, an **E**lectronic **L**ab **N**otebook (ELN) from Radboud University is used:

- **2024-03-19-130946-export.eln**
  Lab notebook from experiment that measures the CMC concentration of SLES from the Boltjes lab. Ultimately to verify if the now adjusted Python script for 1 surfactant runs.

Step 1: Upload file or folder

For this step, a choice between a single file, or multiple folders have to be made. In this test, a single ELN file is uploaded.

A new upload of a single file or zip can be created from shell command:

```
curl -X POST "http://localhost/nomad-
oasis/api/v1/uploads?token=KmGqpha6Tfy7fZ9zATFQKg.T2QHB0ifQ8O7JSW6je

lTVrBi-Q4" -T <Local File>
```

Command 1: Single file upload shell

```
C:\Users\larsv>curl -X POST "http://localhost/nomad-oasis/api/v1/uploads?token=KmGqpha6Tfy7fZ9zATFQKg.T2QHB0ifQ8O7JSW6je
lTVrBi-Q4" -T "D:\SynologyDrive\School ICT\Master s2\data\Radboud\2024-03-19-130946-export.eln"

Thanks for uploading your data to nomad.
Go back to http://localhost/nomad-oasis/gui and press
reload to see the progress on your upload
and publish your data.
```

Figure 7: CMD Response uploading single file

Step 2: Review file structure.

After files are uploaded, they can be viewed in folder structure as uploaded. The GUI gives the possibility to preview the uploaded file. Review all files and make sure there are no errors.

I uploaded an export of eLabFTW, which contained a ro-crate-metadata.json file, which contains metadata extracted by eLabFTW.

The folder of 2024-02-07 – AULAB_PSP0003 – eec0c1d6 contains images and raw json data of the experiment.

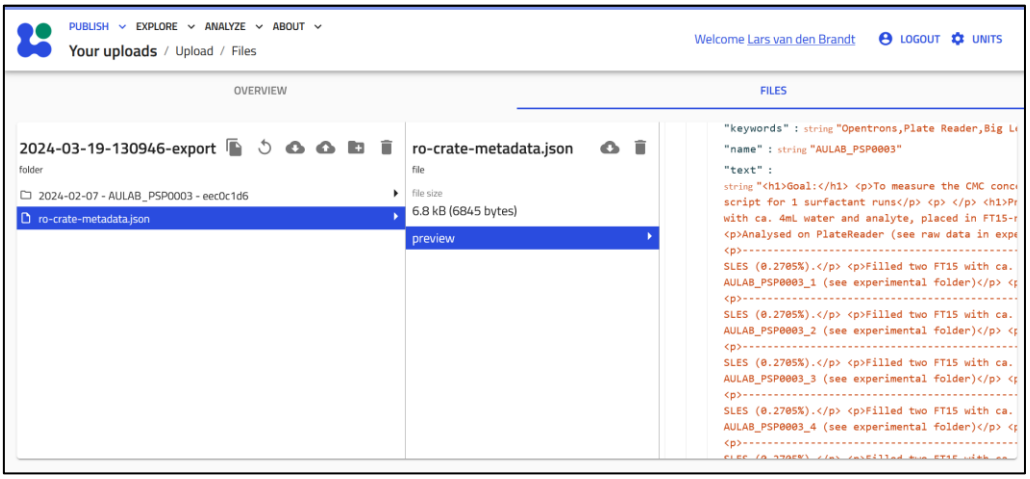

Figure 8: Review file structure

Conclusion

This research explores and documents the diverse range of file types generated by experiments in the realms of Supramolecular and Inorganic chemistry, with a primary focus on data originating from use cases of experiments for the RobotLab project. Through collaboration with the partner universities Radboud University and TU/e together with literature study, insights into the various and voluminous data produced in experiments is created.

Addressing the first question regarding the data formats generated by the RobotLab project, this research has identified a various file types including text files, comma-separated values, videos, images, spectra files, tabular data, and chemical structure files. These formats encapsulate various aspects of experimental data, ranging from raw numerical outputs to visual representations and molecular structures.

The second question regarding the anticipated volume of data generated by the RobotLab project was assessed. Through examination of both experimental data from partner universities and supplementary data from published research, it is concluded that the volume of data can vary significantly depending on the nature of the experiment. However, within the limitations of NOMAD's upload capacity, the study has confirmed that the anticipated data volumes remain manageable.

Finally, in addressing the third question concerning the compatibility of NOMAD Oasis with the diverse data types expected from the RobotLab project. While NOMAD supports the file types and file volume examined in this study, it's noted that parsing raw data into understandable formats may require custom parsers. Despite this challenge, NOMAD's architecture allows for the development of custom parsers to ensure compatibility with the unique data generated by the RobotLab project.

In conclusion, this research has provided an understanding for the data generated in experiments, particularly in the context of the RobotLab project. By clarifying the formats, volumes, and compatibility considerations of this data, the study contributes valuable insights towards the approval of NOMAD’s compatibility for the RobotLab project.

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Table of tables

Table of figures