

## Towards Scalable Algorithms for Neuro-Symbolic AI (CELSA)

### Research Data Summary

List and describe all datasets or research materials that you plan to generate/collect or reuse during your research project. For each dataset or data type (observational, experimental etc.), provide a short name & description (sufficient for yourself to know what data it is about), indicate whether the data are newly generated/collected or reused, digital or physical, also indicate the type of the data (the kind of content), its technical format (file extension), and an estimate of the upper limit of the volume of the data.

Dataset name / ID	Description	New or reuse	Digital or Physical data	Data Type	File format	Data volume	Physical volume
		Indicate: <i>N</i> (ew data) or <i>E</i> (xisting data)	Indicate: D(igital) or P(hysical)	Indicate: Audiovisual Images Sound Numerical Textual Model SOftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
ChemDB	Molecules	E	D	Molecules / Smiles	Text	<100GB	
Algorithm implementations	Implementations of the developed algorithms	Generate new data	Digital	Software	.py	<100MB	

If you reuse existing data, please specify the source, preferably by using a persistent identifier (e.g. DOI, Handle, URL etc.) per dataset or data type:

<https://doi.org/10.1093/bioinformatics/bti683>

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? If so, refer to specific datasets or data types when appropriate and provide the relevant ethical approval number.

- No

Will you process personal data? If so, please refer to specific datasets or data types when appropriate and provide the KU Leuven or UZ Leuven privacy register number (G or S number).

- No

Does your work have potential for commercial valorization (e.g. tech transfer, for example spin-offs, commercial exploitation, ...)? If so, please comment per dataset or data type where appropriate.

- No

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material or Data transfer agreements, Research collaboration agreements)? If so, please explain in the comment section to what data they relate and what restrictions are in place.

- No

Are there any other legal issues, such as intellectual property rights and ownership, to be managed related to the data you (re)use? If so, please explain in the comment section to what data they relate and which restrictions will be asserted.

- No

#### Documentation and Metadata

Clearly describe what approach will be followed to capture the accompanying information necessary to keep data understandable and usable, for yourself and others, now and in the future (e.g. in terms of documentation levels and types required, procedures used, Electronic Lab Notebooks, README.txt files, codebook.tsv etc. where this information is recorded).

Each newly introduced dataset will be accompanied with a README file that contains an explanation of the file structure and the content of each of the fields in the different files.

With each paper published within the context of this project, a runnable notebook or script will be provided that allows reproducing the experiments.

Will a metadata standard be used to make it easier to find and reuse the data ?

If so, please specify which metadata standard will be used.

If not, please specify which metadata will be created to make the data easier to find and reuse.

- Yes

The research is algorithm-oriented. The code will be shared according to the standards in our field. Typically, our algorithms are implemented in python and will then be shared in the the form of an easily installable python package.

#### Data Storage & Back-up during the Research Project

Where will the data be stored?

- Other (specify below)

Software will be developed in KU Leuven GitLab or private GitHub repositories

Datasets will be stored either on the gitlab repositories or the NetApp-based storage solution at the Dept. of Computer Science (KU Leuven).

How will the data be backed up?

- Standard back-up provided by KU Leuven ICTS for my storage solution
- Personal back-ups I make (specify below)
- Other (specify below)

GitLab and the NetApp-based storage system have secure backups that are automatically stored at a second location at KU Leuven, so loss of data is minimized.

Personal backups of the code on the private GitHub repositories will be maintained.

**Is there currently sufficient storage & backup capacity during the project?**

**If no or insufficient storage or backup capacities are available, explain how this will be taken care of.**

- Yes

**How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?**

Only authorized users can access the NetApp-based storage, GitLab repositories and private GitHub repositories.

**What are the expected costs for data storage and backup during the research project? How will these costs be covered?**

All storage and backup costs are covered by the project budget. After the project has ended, the costs will be covered by the DTAI research group.

**Data Preservation after the end of the Research Project**

**Which data will be retained for 10 years (or longer, in agreement with other retention policies that are applicable) after the end of the project?**

**In case some data cannot be preserved, clearly state the reasons for this (e.g. legal or contractual restrictions, storage/budget issues, institutional policies...).**

- All data will be preserved for 10 years according to KU Leuven RDM policy

**Where will these data be archived (stored and curated for the long-term)?**

- Other (specify below)

All data will be archived on the NetApp storage service offered by the Department of Computer Science in the form of snapshots of all text, source code, data and presentations.  
The datasets are also available online.

**What are the expected costs for data preservation during the expected retention period? How will these costs be covered?**

All storage and backup costs are covered by the project budget. After the project has ended, the costs will be covered by the DTAI research group.

## Data Sharing and Reuse

**Will the data (or part of the data) be made available for reuse after/during the project?**  
Please explain per dataset or data type which data will be made available.

- Yes, as open data

The software implementation and artificial datasets will be made available upon publication of the corresponding papers.

**If access is restricted, please specify who will be able to access the data and under what conditions.**

This will be determined throughout the course of the project on the basis of the particular datasets.

**Are there any factors that restrict or prevent the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?**

Please explain per dataset or data type where appropriate.

- No

**Where will the data be made available?**

If already known, please provide a repository per dataset or data type.

- Other data repository (specify below)

The software implementations will be made publicly available through GitHub repositories, as is common practice in our field. The novel components of the artificial datasets will be made available in GitHub repositories, alongside code to properly integrate it with the existing datasets.

**When will the data be made available?**

- Upon publication of research results

**Which data usage licenses are you going to provide?**

If none, please explain why.

- GNU GPL-3.0 (code)
- CC-BY 4.0 (data)
- MIT licence (code)
- Other (specify below)

Permissive licenses. For software, this will be MIT, BSD, GNU or Apache 2.0. For other data, this will be CC-BY-4.0.

**Do you intend to add a persistent identifier (PID) to your dataset(s), e.g. a DOI or accession number? If already available, please provide it here.**

- No

For software, we use the DOI of the relevant publication. The publication details where the code can be downloaded.

**What are the expected costs for data sharing? How will these costs be covered?**

Negligible. All storage and backup costs are covered by the DTAI research group.

#### **Responsibilities**

**Who will manage data documentation and metadata during the research project?**

The PhD and Postdoctoral researchers working on this project

**Who will manage data storage and backup during the research project?**

The PhD and Postdoctoral researchers working on this project

**Who will manage data preservation and sharing?**

Giuseppe Marra will be responsible for ensuring data preservation and reuse during the project.

**Who will update and implement this DMP?**

Giuseppe Marra will update and implement this DMP.