Digestion-based meal design for people living with obesity: Taking the in vitro - in silico - in vivo challenge

FWO DMP (Flemish Standard DMP)

1. 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.

	Only for digital data	*Only for digital data*	*Only for digital data*	*Only for physical data*			
Dataset Name	Description	New or Reused	Digital or Physical	Digital Data Type	Digital Data Format	Digital Data Volume (MB, GB, TB)	Physical Volume
Existing data	Published data for use in literature review	Reuse existing data	Digital	Numerical Textual Model Other: Compiled/aggregated data	.pdf .csv	< 1 GB	
WP1: *In vitro* digestion of meals relevant for people with obesity							
Task 1.0: Strategic design of meals with distinct starch (micro)structural organizations	- Design of meals with identical macronutrient and caloric load but different structural organization	Generate new data	Digital	Numerical Textual	csv .docx	< 1 GB	
- Meal component and meal generation	Generate new data	Physical				Storage at -40 °C (1 small freezer unit)	
- Structural (microstructure, particle size distribution), compositional, and rheological characterization	Generate new data	Digital	Images Numerical Textual	.jpeg .tiff .csv .docx	< 1 GB		
Task 1.1:Understanding interactions between co-ingested meal components	- Static *in vitro* macronutrient digestion kinetics of 8 meal components and 15 combined meals	Generate new data	Physical				Storage at -40 °C (2 large freezer units)

- Characterization of the digesta: *(i)* starch metabolites (HPLC-ELSD), *(ii)* protein metabolites (SEC-HPLC), (iii) rheological, and (iv) microstructural properties	Generate new data	Digital	Images Numerical Model Software	.pdf .csv .jpeg .tiff .sas .jmp	< 1 GB		
Task 1.2: Perspectives of nutrient microstructural organization within meals to impact in vitro digestion kinetics	- Development of semi-dynamic *in vitro* digestion model adapted to digestion conditions of people with obesity	Generate new data	Digital	Numerical Textual Model Software	.pdf .csv .docx .dat	☒ < 1 GB	
- Semi-dynamic *in vitro* digestion of 3-5 meals under semi-dynamic conditions adapted to people with obesity	Generate new data	Physical Digital	Software	.dat		Storage at -40 °C (2 large freezer units)	
- Characterization of the digesta: *(i)* starch metabolites (HPLC-ELSD), *(ii)* protein metabolites (SEC-HPLC), (iii) rheological, and (iv) microstructural properties	Generate new data	Digital	Images Numerical Model Software	.pdf .csv .jpeg .tiff .sas .jmp	< 1 GB		
WP2: Development of an *in silico* model to translate *in vitro* data to *in vivo* data							
Task 2.1: Stepwise development of mathematical model through use of existing data set	- Building of initial *in silico* mathematical model	Reuse existing data Generate new data	Digital	Numerical Model Software	.pdf .csv .sas .jmp	< 100 GB	
Task 2.2: Improving the predictive value of the model using experimental in vitro and in vivo meal data	- Expansion of model based on additional physiological factors	Generate new data	Digital	Model Software	.pdf .csv .sas .jmp	< 100 GB	
WP3: *In vivo* response of people with obesity to distinctly structured meals							
Task 3.1: Semi-dynamic *in vitro* digestion of distinctly structured meals	Semi-dynamic *in vitro* digestion of 3-meals (selected for *in vivo* trial) under semi-dynamic conditions adapted to people with obesity	Generate new data	Physical Digital	Software	.dat		Storage at -40 °C (1 large freezer unit)

Characterization of the digesta: *(i)* starch metabolites (HPLC-ELSD), *(ii)* protein metabolites (SEC-HPLC), (iii) rheological, and (iv) microstructural properties	Generate new data	Digital	Images Numerical Model Software	.pdf .csv .jpeg .tiff .sas .jmp	< 1 GB		
Task 3.2: Evaluation of *in vivo* physiological response to ingestion of test meals in people with obesity	- Blinded, randomized, crossover study of in vivo blood samples upon ingestion of three isocaloric test meals	Generate new data	Physical				Storage at -80 °C? (1 large freezer unit)
- Subjective satiety evaluation (using VAS scales) upon ingestion of three isocaloric test meals	Generate new data	Digital	Images Numerical Textual Other: digitalized VAS sheets	.pdf .csv .sav .jmp	< 1 GB		
- Analysis of blood samples (blood glucose, satiety hormone secretion)	Generate new data	☒ Digital ☐ Physical	☐ Audiovisual ☐ Images ☐ Sound ☒ Numerical ☐ Textual ☒ Model ☒ Software ☐ Other:	.csv .sav .jmp	< 1 GB		
- Hedonic food intake (*ad libitum*) 2h after test meal ingestion	Generate new data	☒ Digital	☒ Numerical	.csv .sav .jmp	< 1 GB		

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:

- - Literature information might be combined at the level of a literature review papers. Of course, at that level, literature sources will be always cited by references as part of the text.
- *The in vitro* digestion model mimicking people with obesity will be based on literature data (which will always be properly cited), existing data at NMAD (https://doi.org/10.1016/j.ejpb.2021.07.002). Enzyme activities in the different phases of the gastrointestinal tract will be obtained from a parallel project within the copromoter's laboratory (NMAD), i.e. Target Digest project funded by VLAIO grant nr. HBC.2023.0244.
- The data set employed for Task 2.1 was obtained both within NMAD and LFT. Therefore, the promotor and copromotor hold the rights to reuse these data.

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? Describe these issues in the comment section. Please refer to specific datasets or data types when appropriate.

- Yes, human subject data

A human trial is planned in Task 3.2. Ethical approval by EC will be applied for in 2nd project year (S-number is not yet available). Informed consent forms will be provided to the participants. Collected personal data will include sex, age, weight, height (and BMI), waist and hip circumference, blood pressure, bioelectrical impedance, resistance, and reactance. These personal data will

be pseudonymized and stored in separated files from the results data (blood glucose and satiety hormones, subjective satiety, and hedonic food intake evaluation). Data will be stored on secured KU Leuven network drives and are only accessible to researchers responsible for the data collection.

Will you process personal data? If so, briefly describe the kind of personal data you will use in the comment section. Please refer to specific datasets or data types when appropriate.

- Yes

See above. The S-number is not yet available.

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/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

2. 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).

Physical data:
A descriptive file indicating where each sample or material is stored will be maintained as a *.xlsx or *.docx file.

Digital data:
- Protocols/experimental and evaluation procedures will be clearly written and maintained in *.docx /*.pdf format.
- Meaningful and descriptive data file names will be used for raw data as well as analyzed data.
- Where initial raw data is exported into a new format: reference to initial data (location) will be made.
- Steps involved in data analysis and relevant analysis will be documented in *.docx file.
- For published material, a metadata will be available: with folders showing the published material, associated processed and raw data files (see below).

Will a metadata standard be used to make it easier to find and reuse the data? If so, please specify (where appropriate per dataset or data type) which metadata standard will be used. If not, please specify (where appropriate per dataset or data type) which metadata will be created to make the data easier to find and reuse.

- Yes

For each published article, a metadata file will be created to ease data retrieval and reuse. This metadata will be based on the Dublin core metadata standard.
The metadata and the referenced files will be stored on the Archive/'K:' network drive. The metadata file will be named based on the title of article, authors, year of publication. Files will include:
- The accepted version of the article as available in KU Leuven, Lirias: *.pdf file.
- The published article as available online in the peer reviewed journal: *.pdf file; wherein doi-number, journal of publication and abstract, etc can be found.
- The peer review history of the article; comments from reviewers, rebuttal to the reviewers: *.pdf file/*.docx.
- An excel sheet of the data used to generate the graphs and tables presented in the published article: *.xlsx.
- A folder (only for internal use) with all excel sheets (*.xlsx) related to the final graphs in the article. In this folder, raw data (including the equipment used, location of the raw/equipment generated data) as well as final data will be referenced.

3. Data storage & back-up during the research project

Where will the data be stored?

- Shared network drive (J-drive)
- Personal network drive (I-drive)
- OneDrive (KU Leuven)
- Sharepoint online
- Archive/'K' network drive will be used when personnel is leaving the research unit. (see use of metadata standard)

How will the data be backed up?

Standard back-up provided by KU Leuven ICTS for my storage solution

Is there currently sufficient storage & backup capacity during the project? If yes, specify concisely.
If no or insufficient storage or backup capacities are available, then explain how this will be taken care of.

- Yes

50 GB of Personal/'I:' data storage for every researcher is available in our research unit. In addition, 2 TB of OneDrive for Business storage space is available for free to every PhD researcher.
1.3 TB of long-term data storage is available on the Archive/'K:' network drive folders of the research unit.
If necessary, more storage space will be acquired from the university, with the cost being covered by the research unit/the bench fee

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

- Data stored on the Personal/'I:' network drive is only accessible to a specific researcher. This data is automatically backed up by ICTS, KU Leuven. Access to KU Leuven network drives is automatically secured by multifactor authentication.
- Data stored on OneDrive for Business is only accessible to a specific researcher. Version history (up to 100 versions per file) is enabled. Multifactor authentication can be activated as an additional security measure. OneDrive for Business will not be used for strictly confidential or personal data.
- Final data files (e.g. see metadata standard) can also be stored on the Archive/'K:' network drive, which has restricted access (only professors and postdocs of the research group).
- Storage of personal data and corresponding coding will be restricted to the Personal/'I:' network drive of the person(s) dedicated to that work package or on the Archive/'K:' network drive which has restricted access (only professors and postdocs of the research group). Access to KU Leuven network drives is automatically secured by multifactor authentication.

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

Storage capacity (on the Archive/'K:' network drive) can be increased for an annual fee of 100.86 Euro/TB. This data is automatically backed up by ICTS, KU Leuven.
Buying additional storage capacity can be covered by the research unit/bench fee.

4. Data preservation after the end of the research project

Which data will be retained for at least five 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
- Only physical samples that are difficult to regenerate will be retained after the end of the project.
- All digital data will be retained for more than the expected 5-year period, on the Archive/'K:' drive.

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

The data will be copied to the Archive/'K:' network drive (with automatic back-up procedures) and stored for at least 10 [A1] years. To date, 1.3 TB storage is available, however if needed, additional data space can be obtained.

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

Annual fee of 100.86 Euro/TB. Research unit budget/the bench fee will be used to cover this cost.

5. Data sharing and reuse

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

- Yes, in a restricted access repository (after approval, institutional access only, …)

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

- Only researchers and professors participating in the project will have access to the data prior to data publication.
- Access of data will be through peer reviewed journals, conference presentations and proceedings, repositories.
- Open access opportunities (major focus on green open access routes) will be considered to enhance visibility of our research.

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 in the comment section 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.

- KU Leuven RDR: Data of completed work will be published in academic peer reviewed journals and will as such be available in existing and relevant repositories (e.g. the internal KU Leuven repository Lirias).
- Open access opportunities (major focus on green open access routes) will be considered to enhance visibility of our research.
- Unpublished data will be available on network drives with restricted access (as explained earlier).

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.

CC-BY 4.0 (data)
Data Transfer Agreement (restricted data)
MIT licence (code)

Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, you have the option to provide it in the comment section.

- No

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

- Within the research unit: the Shared/'J:' network drive will be used and this is freely accessible to all researchers.
- Between collaborating research units: the Shared/'J:' network drive (within KU Leuven) or OneDrive for Business (external partners) will be used.
- Within KU Leuven: Lirias (a free document repository) will be used.
- External data sharing through publication in peer reviewed journals.
- Cost of data sharing at conferences will be covered by the bench fee.
- Cost for possible golden open access will be covered by the bench fee.

6. Responsibilities

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

Dorine Duijsens

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

Dorine Duijsens

Who will manage data preservation and sharing?

During the project: Dorine Duijsens After completion of the project: prof. Tara Grauwet

Who will update and implement this DMP?

During the project: Dorine Duijsens After completion of the project: prof. Tara Grauwet