Bridging the Gap

Molecular Biology DMP catalog creation

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Who are we?

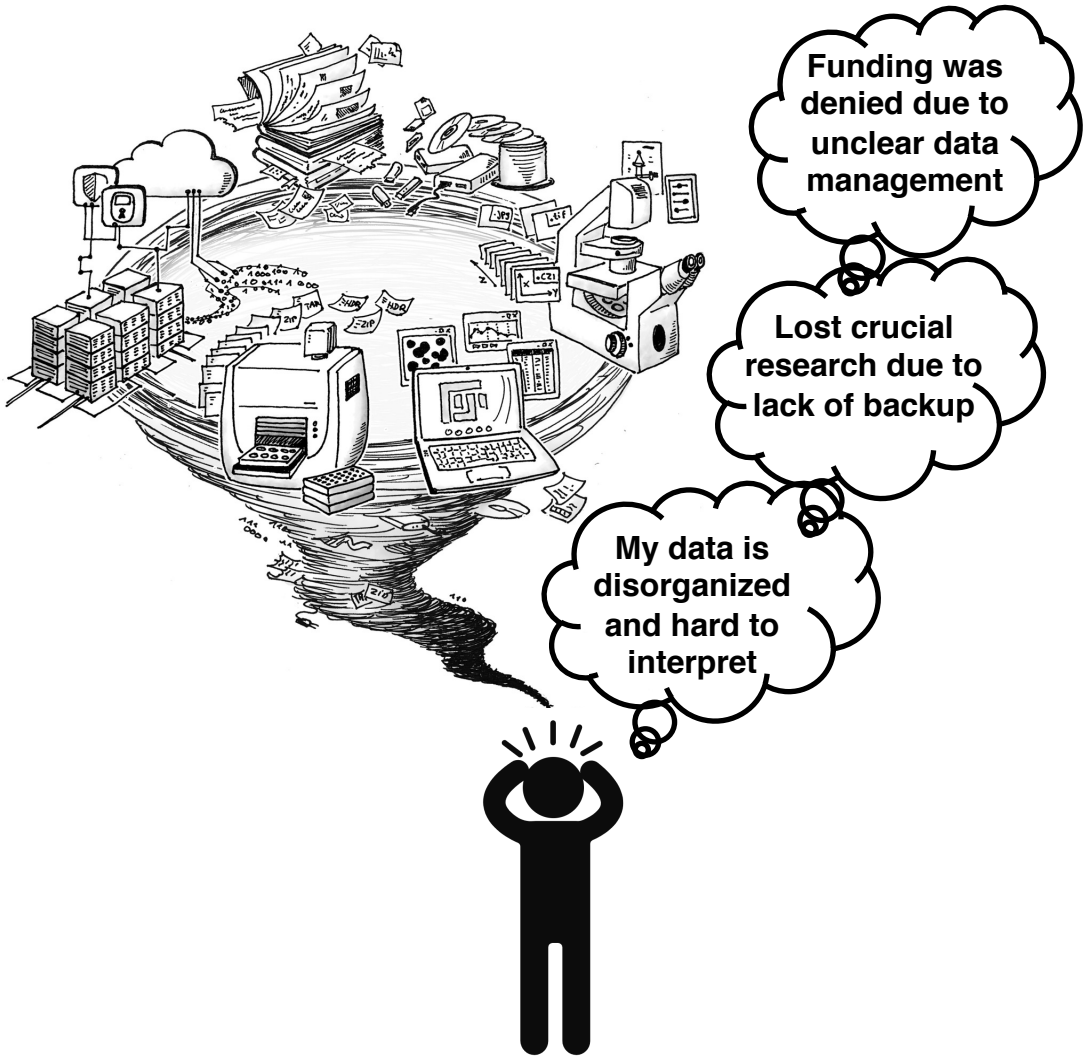
SFB 1361: REGULATION OF DNA REPAIR & GENOME STABILITY

- Data Manager since March 2023
- PhD in Molecular Biosciences

SFB 1551: POLYMER CONCEPTS IN CELLULAR FUNCTION

- Data Manager since June 2023
- 3.5 years research experience in Polymer Physics
- MSc in Computer Science

Effective Data Management: Essential for Successful Research



The Need for Better Guidance

Data management as a fundamental role

- ✓ Equal importance to data generation and analysis.
- ✓ Embrace data management as a researcher.
- ✓ Acknowledge that data management is a fundamental part of your role.

Lack of support and training

- ○ There is a prevailing assumption that researchers should navigate these areas independently.
- ○ Researchers often lack adequate support and training in project and data management.
- ○ Need for detailed and relevant guidance

Promoting RDM Practices and Collaboration in SFBs and IMB

IMPACT

Increase awareness about RDM in SFBs and IMB.

Make RDM practices a regular aspect of scientists' work.

Provide all scientists with comprehensive RDM workshops.

Address data-sharing challenges by implementing comprehensive strategies.

Carry out streamlined data management using DMPs.

Train scientists to create effective DMPs using RDMO tool.

Navigating Challenges and Enhancing DMP Support Through Collaboration

Carry out streamlined data management using DMPs.

Train scientists to create effective DMPs using RDMO tool.

How ?

✓ **Part of the institutional and SFB policy to submit DMP**

RDM Supports Researchers Throughout the Data Lifecycle

DMPs serve as the first step in the RDM life cycle

DMP Realities: Scientists' Expectations vs. Practical Insights

Expectations

- Data handling solutions in research projects
- Aiding researchers' daily tasks

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Reality

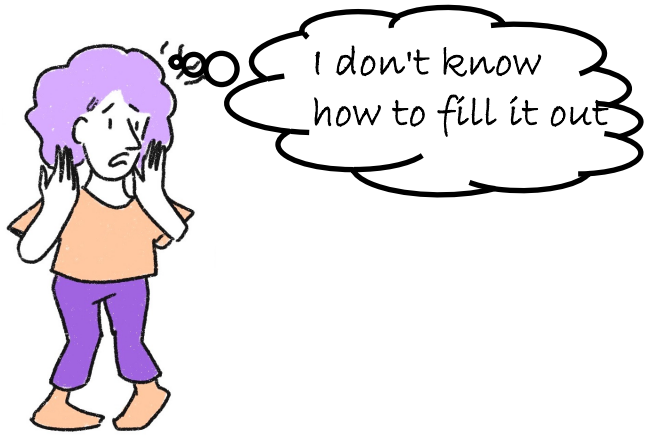
- Generic and lacks specific guidance
- Tedious and bureaucratic
- Requirement for grant approval

DMP Realities: Scientists' Expectations vs. Practical Insights

Expectations

- Data handling solutions in research projects
- Aiding researchers' daily tasks

Reality



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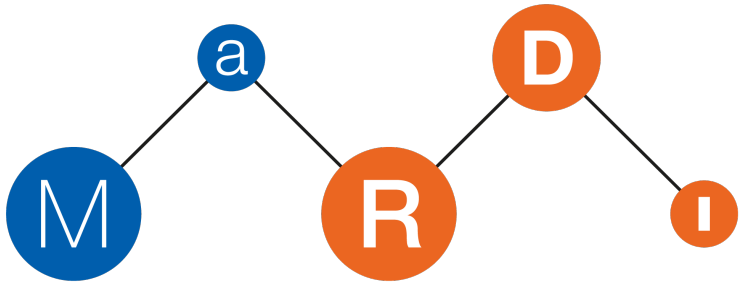
Aim

- Discipline-appropriate guidance and improved answering options
- Assists researchers in their day-day work
- Greater satisfaction with DMPs

RDM Working Groups with Tailored DMPs

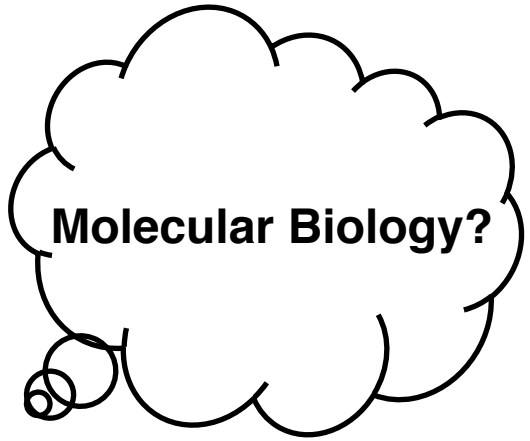
Adapted DMPs of some existing initiatives in various disciplines, for example in Chemistry, Biodiversity and Engineering using RDMO.



DMP Tools: An Overview

Table 1: Evaluated DMP tools. Discipline-specific tools are marked in light green.

DMP tool	Discipline	Hosting/Developers
ARGOS	Interdisciplinary	OpenAIRE AMKE, EUDAT CDI, Europe
ARIADNE	Archeology	Vast-Lab, Italy
Clarin-d DMP	Humanities/social sciences	Eberhard Karls Universität Tübingen, Germany
Data Stewardship Wizard	Interdisciplinary	Czech Technical University, Dutch Techcentre for Life Sciences, Czech Republic, Netherlands
DataWiz	Psychology	Leibniz Institute for Psychology Information, Germany
DMP Canvas Generator	Life sciences	Swiss Institute of Bioinformatics, Switzerland
DMPonline	Interdisciplinary	Digital Curation Centre, University of Edinburgh, United Kingdom
DMPTool	Interdisciplinary	California Digital Library, University of California, USA
easyDMP	Interdisciplinary	EUDAT, Finland, Norway
ezDMP	Interdisciplinary	Columbia University, Rutgers University, University of Illinois, USA
GFBio	Biodiversity	GFBio, Germany
NFDI4Plants DataPLAN	Plant science	Eberhard Karls Universität Tübingen, Germany
QUT	Interdisciplinary	Queensland University of Technology, Australia
RDMO	Interdisciplinary	Leibniz Institute for Astrophysics Potsdam, University of Applied Sciences Potsdam, Germany
RDMO NFDI4Ing	Engineering	University and State Library Darmstadt, Germany
TUDD DMP	Interdisciplinary	TU Dresden, Germany
TUM Workbench	Interdisciplinary	TU München, Germany
UWA-DMP	Interdisciplinary	University of Western Australia, Australia



https://zenodo.org/records/8369596

Challenges with Current Data Catalogs in Molecular Biology

Lacks informative guidance and overly generalized

- The content is too generic and lacks specificity
- Absence of helpful explanations and guidance
- Specific examples are needed for better understanding

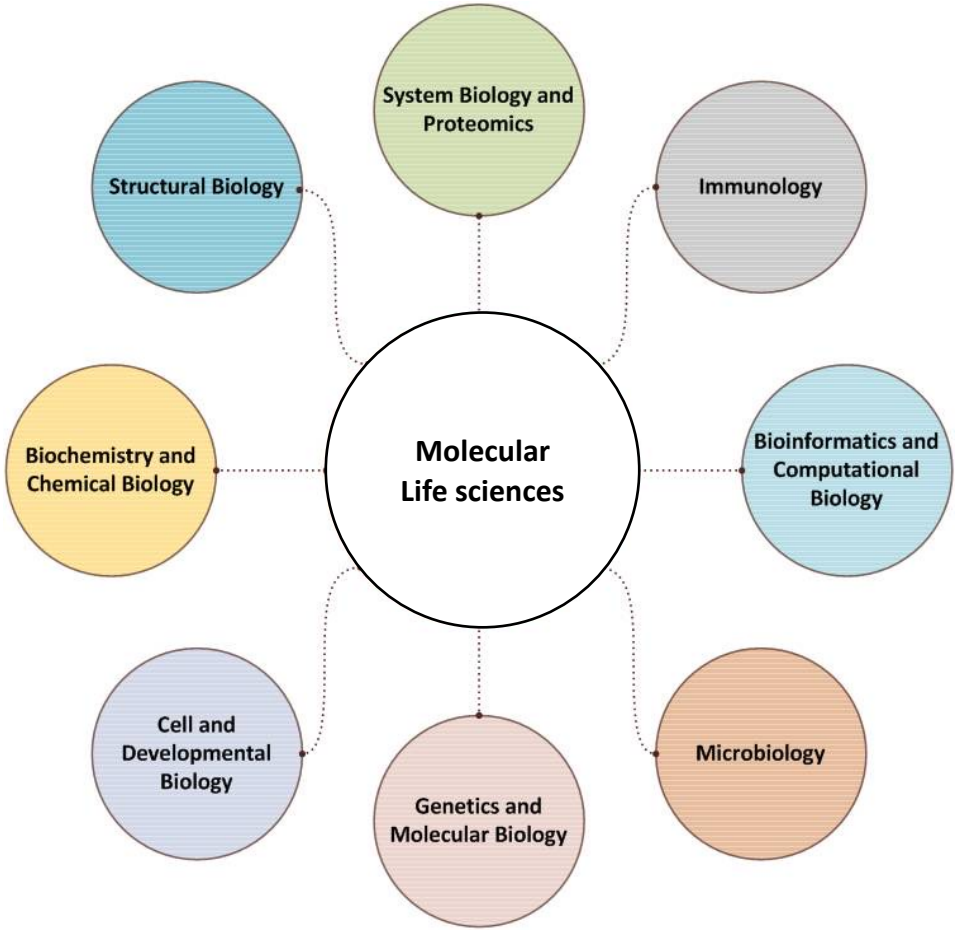
Discipline vs. data type classification

- Current classification is based on research disciplines
- Our approach aims to classify based on data types
- Molecular biology involves numerous subdisciplines; projects often span multiple areas

Addressing Challenges in Molecular Biology Catalog Creation

1

Interdisciplinary research projects encompass various sub-disciplines with unique research focuses



Addressing Challenges in Molecular Biology Catalog Creation

2

Different sub-disciplines have distinct data requirements

Engineering Sciences

- NFDI4DataScience: NFDI for Data Science and Artificial Intelligence
- NFDI4Energy: National Research Data Infrastructure for Interdisciplinary Energy System Research
- NFDI4Ing: NFDI for Engineering Sciences
- NFDI-MatWerk: National Research Data Infrastructure for Materials Science and Materials Engineering
- NFDIxCS – National Research Data Infrastructure for and with Computer Science

nfdi Nationale Forschungsdaten Infrastruktur

Life Sciences

- DataPLANT: Plant research data
- FAIRagro: FAIR Data Infrastructure for Agrosystems
- NFDI4Immuno – National Research Data Infrastructure for Immunology
- GHGA: National Research Data Infrastructure for Immunologyv
- NFDI4Biodiversity: Biodiversity, Ecology and Environmental Data
- NFDI4BIOIMAGE: National research data infrastructure for microscopy and bioimage analysis
- NFDI4Health: NFDI personal health data
- NFDI4Microbiota: NFDI for Microbiota Research

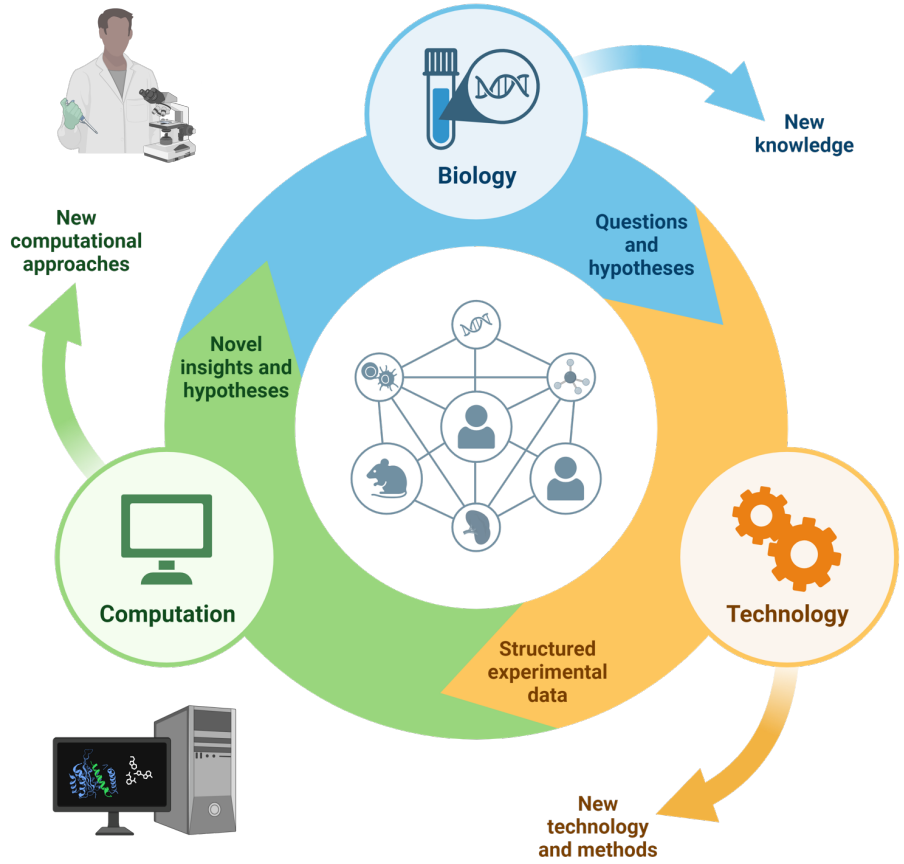
Natural Sciences

- DAPHNE4NFDI: Data from PHoton and Neutron Experiments for NFDI
- FAIRmat: FAIR Data Infrastructure for Condensed-Matter Physics and the Chemical Physics of Solids
- NFDI4Cat: NFDI for sciences related to catalysis
- MaRDI: Mathematical Research Data Initiative
- NFDI4Chem: Chemistry consortium for the NFDI
- NFDI4Earth: NFDI Consortium Earth System Sciences
- PUNCH4NFDI: Particles, Universe, NuClei and Hadrons for the NFDI

Addressing Challenges in Molecular Biology Catalog Creation

3

Involves a broad spectrum of data types and methodologies



It is very rare that a DMP would have one dataset

- The specificity of sub-disciplines within molecular biology results in even greater diversity of data types and methodologies.
- Diverse data types
  - Quantitative data: laboratory measurements
  - Qualitative data: textual information and images
  - Physical data: biological specimens, genetic sequences, and experimental records
  - Statistical data: analysis results and statistical models

Created with Biorender.com

Diverse Data Landscape in Molecular Biology

High-Throughput Experiments:

1.Genomic data (e.g., DNA sequences, gene expression profiles, ChIP-seq data)
2.Transcriptomic data (e.g., RNA-seq data, microarray data)
3.Proteomic data (e.g., mass spectrometry data, protein-protein interaction data)
4.Metabolomic data (e.g., metabolite profiles, metabolic flux data)
5.Epigenomic data (e.g., DNA methylation data, histone modification data)
6.High-resolution microscopy images (e.g., confocal microscopy, super-resolution microscopy)
7.Flow cytometry data (e.g., single-cell analysis, cell sorting data)
8.Next-generation sequencing data (e.g., whole-genome sequencing, targeted sequencing)
9.Single-cell sequencing data (e.g., single-cell RNA-seq, single-cell ATAC-seq)
10.CRISPR/Cas9 screening data (e.g., knockout screens, genetic interaction screens)
11.Protein structure data (e.g., X-ray crystallography, NMR spectroscopy)
12.Time-lapse imaging data (e.g., cell migration, cell division)
13.Comparative genomics data (e.g., phylogenetic analysis, gene family evolution)
14.Protein-DNA interaction data (e.g., DNA-binding assays, chromatin immunoprecipitation)
15.Network analysis data (e.g., protein-protein interaction networks, gene regulatory networks)
16.DNA methylation data (e.g., methylation profiles, CpG island analysis)
17.Single-nucleotide polymorphism (SNP) data (e.g., SNP genotyping, association studies)
18.Metagenomic data (e.g., microbial community composition, functional profiling)
19.Pathway analysis data (e.g., enrichment analysis, pathway mapping)
20.Computational modeling and simulation data (e.g., molecular dynamics simulations, protein folding predictions)
21.Bioinformatics analysis outputs (e.g., gene annotations, sequence alignments)
22.Protein expression localization data (e.g., subcellular localization, organelle-specific markers)
23.DNA-protein crosslinking data (e.g., chromatin conformation capture, Hi-C data)
24.RNA secondary structure analysis data (e.g., RNA folding predictions, RNA-RNA interactions)
25.Single-molecule imaging data (e.g., single-molecule fluorescence, single-particle tracking)

Low-Throughput Classical Approaches:

1. Western blot data (e.g., protein expression levels, post-translational modifications)
2. PCR and RT-PCR data (e.g., gene amplification, gene expression analysis)
3. Gel electrophoresis data (e.g., DNA, RNA, or protein separation)
4. Immunohistochemistry and immunofluorescence data (e.g., tissue staining patterns, cellular localization)
5. Histological data (e.g., tissue sections, staining intensity)
6. Enzyme activity assays (e.g., enzyme kinetics, substrate specificity)
7. Cell viability and proliferation data (e.g., cell counting, MTT assays)
8. Reporter gene assays (e.g., luciferase assays, beta-galactosidase assays)
9. Protein purification data (e.g., protein yield, purity, activity)
10. Microbial growth data (e.g., growth curves, colony-forming units)
11. Tissue culture data (e.g., cell passage number, cell morphology)
12. Cell migration and invasion assays (e.g., scratch assays, transwell assays)
13. DNA footprinting data (e.g., protein-DNA interaction analysis)
14. Mutagenesis data (e.g., site-directed mutagenesis, functional characterization)
15. Cell cycle analysis data (e.g., DNA content analysis, cell cycle phase determination)
16. Knockdown or knockout data (e.g., siRNA experiments, CRISPR/Cas9-mediated gene knockout)
17. Enzyme kinetics data (e.g., Michaelis-Menten analysis, Lineweaver-Burk plots)
18. Ligand-receptor binding data (e.g., binding affinity, dissociation kinetics)
19. DNA/RNA hybridization data (e.g., in situ hybridization, northern blot)
20. Cell signaling pathway analysis data (e.g., phosphorylation cascades, signal transduction)
21. Metabolic flux analysis data (e.g., stable isotope labeling, metabolic network modeling)
22. Protein-protein interaction data (e.g., yeast two-hybrid, co-immunoprecipitation)
23. Cell adhesion and migration data (e.g., scratch wound healing, transmigration assays)
24. Ion channel electrophysiology data (e.g., voltage-clamp recordings, current-voltage relationships)
25. Hormone or ligand response data (e.g., dose-response curves, signal transduction pathways)

Addressing Challenges in Molecular Biology Catalog Creation

4

Data handling at different levels.
The lack of existing guidelines creates standardization issues for scientists.

High throughput Core facilities at IMB

DIRECTOR OF CORE FACILITIES	BIOINFORMATICS	FLOW CYTOMETRY
GENOMICS	HISTOLOGY	MICROSCOPY
PROTEOMICS	PROTEIN PRODUCTION	MEDIA LAB
E-LAB	CORE FACILITIES LECTURES	CORE EQUIPMENT

Addressing Challenges in Molecular Biology Catalog Creation

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Interdisciplinary research projects encompass various sub-disciplines with unique research focuses.

2

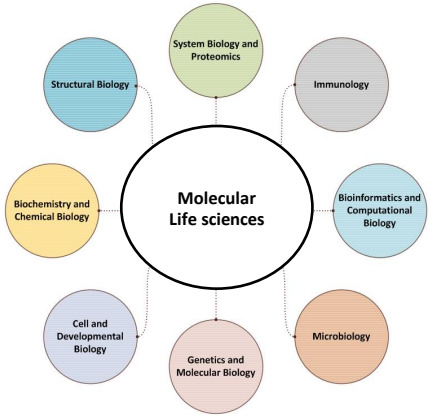
Different sub-disciplines have distinct data requirements.

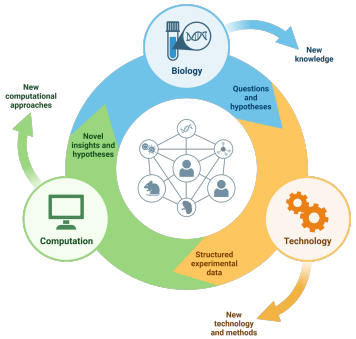
3

Involves a broad spectrum of data types and methodologies.

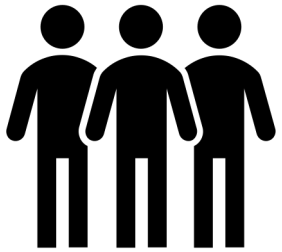
4

Data handling at different levels. The lack of existing guidelines creates standardization issues for scientists.





First Steps to Molecular Biology and Institutional-Specific DMP Templates



- Work with team of PIs at the institute to discuss current DMP and propose modifications

- Follow the same steps as the **discipline specific WG guidelines**

Offer Guidance by Providing Suitable Answer Options

Datasets

Current question

The following questions collect information on the data that is produced or used in the project. They also help to estimate the value of the data in terms of potential re-use and long-term preservation. Before data is newly created, it is advisable to check if there is existing data that could be re-used. This way, redundant collection or creation of research data is prevented. This saves efforts and costs.

Please fill in the form for each dataset. The different datasets will be referred to in following questions. You can add a new dataset using the green button. Once created, you can edit or delete datasets using the buttons in the top right corner.

Dataset 1 | Add dataset

What kind of dataset is it?

Please briefly describe the data type and / or the method used to create or collect the data, for example: * quan
3D model / digital reconstruction of a stone age settlement * software developed within the project

Proposed adjustment

What kind of dataset is it?

Please choose the data type and / or the method used to create or collect the data, for example:

- [ ] Genomic sequencing data (e.g., whole genome, exome)
- [ ] Transcriptomic data (e.g., RNA-Seq, microarrays)
- [ ] Proteomic data
- [ ] Metabolomic data
- [ ] Structural biology data (e.g., X-ray crystallography, NMR)
- [ ] Functional assays (e.g., reporter assays, CRISPR screens)
- [ ] Imaging data (e.g., microscopy, flow cytometry)
- [ ] Biophysical data (e.g., isothermal titration calorimetry, surface plasmon resonance)
- [ ] Computational models and simulations
- [ ] Pathway and network data
- [ ] Others (please specify):

Outlook

Modify first draft of DMP -> aim for the next 6 months

Distribute DMP to researchers

Adjust DMP based on feedback

Share the template publicly

Enhancing the Role of Data Management Plans in Molecular Biology

Current perception

Considered a recent requirement in molecular biology.

DMPs are viewed as paperwork for grant application/approval.

Existing challenges

Current DMPs lack practical usefulness for scientists.

Seen as tedious and bureaucratic tasks.

Proposed solutions

Develop a new DMP model tailored to molecular biology.

Provide practical, project-specific guidance and support.

Enable scientists to effectively manage their research activities.

Expected Benefits:

Empower scientists to navigate their projects more efficiently.

Foster a positive perception of DMPs as valuable tools.

Improve the overall research experience in molecular biology.

Thank you for listening

References

- https://the-turing-way.netlify.app/reproducible-research/rdm/rdm-dmp.html -adjusted the original image
- https://gerbi-gmb.de/2022/06/13/nfdi4bioimage_community_survey/ , https://twitter.com/DrHenningFalk - adjusted the original image
- https://rdmkit.elixir-europe.org/images/data_life_cycle.png
- https://www.mls-phd.uzh.ch/en/Programme-Overview.html
- https://www.rd-alliance.org/
- https://www.nfdi.de/
- https://nfdi4ing.de/
- https://www.nfdi4chem.de/
- https://www.mardi4nfdi.de/about/mission
- https://fodako.nrw/
- https://www.gfbio.org/
- https://fair-wizard.com/
- MS pictograms
- https://www.uni-mainz.de
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