



Project: 101086373 – MET-EFFECT
HORIZON-MSCA-2021-SE-01



Horizon Europe

Data Management Plan Template

Version 1.0
05 May 2021



Funded by the European Union



HISTORY OF CHANGES		
Version	Publication date	Changes
1.0	05.05.2021	<ul style="list-style-type: none">▪ Initial version
		<ul style="list-style-type: none">▪





Action Number: [101086373]

Action Acronym: [MET-EFFECT]

Action title: [Metal complexes of a naturally inspired framework functionalized for cytotoxic and catalytic efficiency]

Date: [31/05/2023]

DMP version: [1.0]



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Metal complexes of a naturally inspired framework functionalized for cytotoxic and catalytic efficiency

D6.1. Data Management Plan

Deliverable Report

Due date: M6

Lead Beneficiary: ICFCB

Dissemination level: PU

Version: 1.0





Project information

Project title: Metal complexes of a naturally inspired framework functionalized for cytotoxic and catalytic efficiency

Project acronym: MET-EFFECT

Consortium members:

1. Innovative Centre Faculty of Chemistry Belgrade Ltd. (Coordinator)
2. Venus Roses Labsolutions Ltd., Bulgaria (Beneficiary)
3. Centiv GmbH, Germany (Beneficiary)
4. UNI GRAZ, Austria (Beneficiary)
5. Associacao do Instituto Superior Tecnico para a Investigacao e Desenvolvimento, Portugal (Beneficiary)
6. Case Western Reserve University, USA (Associated partner)

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Deliverable information

Deliverable: D6.1.

Deliverable title: Data Management Plan

Deliverable description: Data Management Plan

Due date: 30/06/2023

Submission date: 27/06/2023

Lead author: Ljiljana Mihajlović-Lalić, PC

Person responsible for D6.1.: Ljiljana Mihajlović-Lalić, PC

Means of verification: Report



Executive Summary

The document represents the initial Data Management Plan (DMP) for the MET-EFFECT project, funded by the EU's Horizon Europe under Grant Agreement number 101086373. DMP represents a unique guide on how the generated data sets will be collected, prepared, stored, and reused. Moreover, the document utilizes a project data management policy defining the way of managing and sharing data with e.g. third parties.

1. Data Summary

1.1. Will you re-use any existing data and what will you re-use it for? State the reasons if re-use of any existing data has been considered but discarded.

Proper data selection, collection, and unobstructed access to the project data are necessary for achieving well-defined project objectives identified in order to:

(Objective 1). synthesize and fully characterize rationalized metal-based flavonoid complexes (rhenium and iridium).

(Objective 2) - evaluate the anticancer potential of newly synthesized compounds

(Objective 3) - evaluate the catalytic potential of novel complexes

(Objective 4) - develop suitable drug design delivery systems (DDDS) using smart, sustainable biomaterials

(Objective 5) - develop sustainable procedures for metal recycling

(Objective 6) - maximize the overall visibility of MET-EFFECT by targeting three major types of audiences: the scientific community, industry stakeholders, and the general public.

Research data will be generated through the activities performed under scientific objectives O1-5.

It is foreseen to re-use existing literature data for the cause of comparison of spectral data such as descriptions of experimental synthetic procedures; analytical data (NMR, MS, IR, UV-Vis, EA, X-ray), procedures for extracting analytically pure salts of rhenium and iridium from reaction mixtures, cytotoxicity data from in vitro and in vivo studies, literature survey results.

1.2. What types and formats of data will the project generate or re-use?

Project implementation will generate different types of data given in the form of:

- uniform data sheet (hard copy) with a detailed description of reaction conditions, standardized in the chemical literature (.pdf or .doc formats)
- tabular data and metadata (comma separated values format such as .CSV or XML)
- text content data, (.pdf or .doc formats; .odt for the purpose of data storage and dissemination)
- statistical data (.sas7bdat (SAS), .RData (R), .SAV (SPSS), .mat (matlab))
- visual content data (.svg and JPEG 2000 formats)
- other heterogeneous data such as Origin Project and MestreNova will be used as essential tools for regular handling of the generated spectroscopic data on a daily basis (.txt and .CSV format)

1.3. What is the purpose of the data generation or re-use and its relation to the objectives of the project?

The main purpose of data generation and proper data storage reflects in the possibility of transparently accessing experimental results, obtained by performing activities under scientific objectives O1-5. The data will be used for publications, potential patent applications, joint Ph.D. thesis etc. On the other hand, the main purpose of data re-use relies on literature surveys regarding the newest achievements in the field of the project's scientific interests.

1.4. What is the expected size of the data that you intend to generate or re-use?

Depending on the size of the panel of newly synthesized compounds, it is foreseen to generate data up to 1 TB. However, this parameter might vary during the project implementation.

1.5. What is the origin/provenance of the data, either generated or re-used?

The newly generated data will originate from proper databases of all Consortium members developed through different project activities (research, training, communication, dissemination, and managerial activities)

1.6. To whom might your data be useful ('data utility'), outside your project?

MET-EFFECT data will be beneficial for Consortium partners, services of the European Commission, European Agencies, the scientific community, and above all general public.

2. FAIR data

2.1. Making data findable, including provisions for metadata

2.1.1. Will data be identified by a persistent identifier?

The metadata related to the generated research data will be in parallel deposited to Chemotion (www.chemotion.net/chemotionsaurus/index.html) trusted repository as well as to the Cherry, the Institutional Repository of the University of Belgrade-Faculty of Chemistry. ICFCB's members have continuous access to the Cherry. It is foreseen to detail metadata to a large extent. The activity will be performed to enable their trackability alongside their origin and content and further will ensure their smooth identification and proper citation. Both suggested repository services can provide metadata "in the Dublin Core™ style". Additionally, Chemotion Repository for samples, reactions, and related research data is based on DataCite Metadata Scheme. Thus, it is not planned to initiate any new standards for metadata. The Digital Object Identifier (DOI) will be assigned to the research data in Chemotion while in Cherry Handle persistent identifiers will be used.

2.1.2. Will rich metadata be provided to allow discovery? What metadata will be created? What disciplinary or general standards will be followed? In case metadata standards do not exist in your discipline, please outline what type of metadata will be created and how.

In the collaborative research environment, highly diverse project data will be obtained, collected, and spread across participating institutions and repositories, following FAIR principles. It is foreseen to further improve this DMP version according to the project's needs and demands of the European Commission. As mentioned above, the generated data will be deposited to Chemotion (www.chemotion.net/chemotionsaurus/index.html) trusted repository as well as to the Cherry, the Institutional Repository of the University of Belgrade-Faculty of Chemistry. The repositories provide metadata "in the Dublin Core™ style" and have developed OAI-PMH protocol for metadata harvesting. Additionally, both of the repositories store data in a machine-readable way, making the data available under CC licenses. Using both of them will enable researchers to store raw data in the institutional repository while publically available will be stored in Chemotion.

Finally, national coordinators from Consortium institutions will be responsible for data management while ICFCB will be responsible for national depositing.

2.1.3. Will search keywords be provided in the metadata to optimize the possibility for discovery and then potential re-use?

To ensure findable and accessible data, it is foreseen to characterize each data set by proper keywords (dc. subject field) which will reflect the topics of interest. In the proposed repositories, dc. subject elements have keywords that can be tracked by OAI-PMH. Consequently, the stored data is findable and accessible on multiple platforms. MET-EFFECT researchers will put focus on metadata descriptive and structural elements, such as keywords that reflect chemical elements, reactions, analyses, or optional temporal coverage etc. The activity will enable search refinement.

2.1.4. Will metadata be offered in such a way that it can be harvested and indexed?

Regarding the file naming, it will be performed by naming convention which will automatically provide some additional metadata information. Suffixes will also be used to easily track the latest versions stored in a repository. In the Chemotion repository, the uploaded data version will be assigned by DOI. However, this will not be possible in Cherry as it does not support this type of streamlining. In the case of Cherry, the version will be labeled and described with metadata so that multiple versions may be connected via links.

The structure of a well-formed metadata file name will include 3 mandatory parts:

- a prefix that indicates either metadata or dataset/template
- a root consisted of a short but descriptive name of the dataset/template and acronym (for templates is MET-EFFECT by default)
- a suffix reporting the latest date of the upload (in YYYYMMDD format)

The elements will be commonly separated by an underscore symbol, _.

Designed in this way, metadata will be smoothly harvested and indexed.

2.2. Making data accessible

Repository:

2.2.1. Will the data be deposited in a trusted repository?

The institutional repository, <http://cherry.chem.bg.ac.rs>, will be used to deposit data from their raw, primary versions, over their intermediate to final records. For this purpose, a separate



MET-EFFECT segment will be generated. The repository permits operating with quality-controlled data sets and their different versions under the supervision of data owners/providers. A web user interface will allow nominated users/administrators to view metadata and data sets. Consortium representatives will be enabled to approach and deposit their data in an assigned section.

2.2.2. Have you explored appropriate arrangements with the identified repository where your data will be deposited?

The identified repository acts using a technology that supports GDPR regulations. Crucial key metrics that ensure a GDPR-ready platform relies on:

- EU platform and security protocols providing a high level of control
- data accessibility (nominated persons will access and locate data)
- centralized management (as stated above, the selected data will be collected in a single repository accessible by nominated persons)
- data retention (the collected data will be retained under GDPR compliance).

2.2.3. Does the repository ensure that the data is assigned an identifier? Will the repository resolve the identifier to a digital object?

Chemotion supports automated Digital Object Identifier (DOI) generation. The repository creates DOI automatically for accepted submissions enabling the data set to be cited and referenced. Thus, no further operations by data users are necessary. In the case of UBFC Repository – Cherry (meta)data will be assigned Handle persistent identifiers.

Data:

2.2.4. Will all data be made openly available? If certain datasets cannot be shared (or need to be shared under restricted access conditions), explain why, clearly separating legal and contractual reasons from intentional restrictions. Note that in multi-beneficiary projects it is also possible for specific beneficiaries to keep their data closed if opening their data goes against their legitimate interests or other constraints as per the Grant Agreement.

Two repositories will be used for the preservation and sharing of research (meta)data with discipline-specific methods and data processing tools, namely Chemotion and UBFC institutional repository – Cherry. Both of them are free of charge, and the data are provided and licensed as Open Data. Additionally, a dedicated MET-EFFECT data collection in Cherry will be harvested by BASE. The nominated Data Owner in the project will define under which conditions data can be made publicly available. Therefore, the nominated person will ensure data protection, followed by the implementation of policies, guidelines, and memorandums that describe the relevant data usage.

2.2.5. If an embargo is applied to give time to publish or seek protection of the intellectual property (e.g. patents), specify why and how long this will apply, bearing in mind that research data should be made available as soon as possible.

The Chemotion repository has a set up with a rich functionality that enables data providers with manifold functions, such as embargo settings. However, it is foreseen make all publications open-access. In the case of preparing intellectual property document, the results will be closed by the time the draft is submitted but openly accessible as soon as possible.

2.2.6. Will the data be accessible through a free and standardized access protocol?

The use of the repository is free of charge for data providers and is well-defined through standardized procedures (Angew. Chem. Int. Ed. 2020, 59, 22771–22778). The nominated Data Owner will be in charge of data classification (open, restricted, closed, and embargo) as well as for making data publicly available. Considering the conservation of metadata classified as restricted, it will be possible to access it upon a request to Data Owner.

2.2.7. If there are restrictions on use, how will access be provided to the data, both during and after the end of the project?

It is foreseen to protect the experimentally generated data until they are published. The adoptive publishing model of Open Access will be preferred. A significant amount of data will be conserved in a separate segment of Cherry, specifically generated for MET-EFFECT implementation. For open access to research data, Chemotion will be used, relying on standard qualitative and security checkings.

2.2.8. How will the identity of the person accessing the data be ascertained?

The project data workspace in Cherry will be created with the purpose of sharing data between Consortium members. Cherry anticipates accessing the workspace only by a previously defined administrator. The administrator will approve a limited user list that will have restricted access in terms of data upload and download. Other classified data (e.g. personal or budget data) will be accessible only to previously accredited persons.

2.2.9. Is there a need for a data access committee (e.g. to evaluate/approve access requests to personal/sensitive data)?

In the case of an urgent need for personal/sensitive data evaluation/approval, a data access committee will be established. However, at this project stage, it cannot be predicted in advance. Thus, all actions linked to generated/ published data will strictly rely on regulations within the Consortium Agreement.

Metadata:

2.2.10. Will metadata be made openly available and licenced under a public domain dedication CC0, as per the Grant Agreement? If not, please clarify why. Will metadata contain information to enable the user to access the data?

The repository policy defines that authors can publish content under the public domain mark. Data will be available under CC by CC 0 or SA 4.0 license. Open Access to data will be enabled for all interested users, but the download of datasets is limited only to registered users so that potential misuse is avoided.



2.2.11. How long will the data remain available and findable? Will metadata be guaranteed to remain available after data is no longer available?

It is foreseen to make metadata publicly available by default and follow protocol for harvesting publication metadata by OpenAIRE and BASE.

2.2.12. Will documentation or reference about any software be needed to access or read the data be included? Will it be possible to include the relevant software (e.g. in open source code)?

Open data formats will be preferred as much as possible. As the data storage includes domain-specific information, some of the file formats may not be familiar to the wider scientific community. Thus, this type of data will be additionally supported by the corresponding metadata and readme formats. The code of the software will be available via GitHub as Open Source.

Several formats are described below:

- .odt format can be opened in a few ways (applications with native ODF compatibility, MS Office, Google Docs etc.)
- .opj format can be accessed using Origin or Origin Viewer
- .mnova files can be opened by commonly used MestReNova software
- .CSV files offer many choices for opening (MS Excel, Google sheet, Notepad, and OpenOffice Calc)
- .jpg, .tiff, or .png formats can be opened by any image viewer (e.g. MS Photos) or web browser ([Google Chrome](#), [Microsoft Edge](#))
- XML files are easily open in a text editor, web browser, XML viewer, or MS Excel
- .ods or .ots formats can be accessed using OpenOffice.org Calc and Google Docs
- SVG files can be operated by all major browsers (Chrome, Edge, FireFox)

2.3. Making data interoperable

2.3.1. What data and metadata vocabularies, standards, formats or methodologies will you follow to make your data interoperable to allow data exchange and re-use within and across disciplines? Will you follow community-endorsed interoperability best practices? Which ones?

The project actions will strive to achieve data interoperability by exposing the data that can be defined as suitable for most cases. The term interoperability is relative and ranges from general-purpose standards (e.g. Dublin Core) to very specific scientific cases (e.g. data specification). Thus, the project flow will direct the rate and nature of data interoperability. Both targeted repositories (Cherry and Chemotion) guarantee for metadata interoperability.

The interoperability of specific formats is given below:

- .odt format files can be edited using Apache OpenOffice or LibreOffice
- .opj files are defined as interoperable but convertible by a suitable software
- CSV format is compatible and interoperable with other basic file types (e.g. XLS, TXT, and HTML)
- .jpg, .tiff, or .png formats allow interoperability between systems and applications
- XML files are recognized as a format of high-level interoperability since they can be exchanged between heterogeneous and cross-platform systems relying on free open standards



- .ods or .ots formats are generated as designed to be highly portable, interoperable, and editable by e.g. OpenOffice Calc
- SVG files are entirely interoperable and editable by numerous Windows editors (SVG-Edit, [Vecteezy](#) etc.)

2.3.2. In case it is unavoidable that you use uncommon or generate project specific ontologies or vocabularies, will you provide mappings to more commonly used ontologies? Will you openly publish the generated ontologies or vocabularies to allow reusing, refining or extending them?

At this project stage, it is not foreseen to generate project-specific ontologies or vocabularies.

2.3.3. Will your data include qualified references to other data (e.g. other data from your project, or datasets from previous research)?

In case MET-EFFECT data is in any way linked to some other datasets from previous research, the relationship between those datasets in the metadata will be properly identified. The scientific relation will be described by naming the persistent identifier and describing the corresponding scientific link to each other (in a form of e.g. 'the data correlates to', or 'supplements to').

2.4. Increase data re-use

2.4.1. How will you provide documentation needed to validate data analysis and facilitate data re-use (e.g. readme files with information on methodology, codebooks, data cleaning, analyses, variable definitions, units of measurement, etc.)?

The necessary documentation will be provided in a form of readme files as a clear and concise description of all relevant details about data collection, processing, and analysis. This format may be useful for interested researchers in terms of an easy interpretation and reanalyzing stored dataset.

2.4.2. Will your data be made freely available in the public domain to permit the widest re-use possible? Will your data be licensed using standard reuse licenses, in line with the obligations set out in the Grant Agreement?

It is foreseen to make the generated data publicly accessible right after the publication is accepted, relying on universal public domain (CC0 and CC BY). The targeted types of licences are distinguished by their universal form, open sharing, and possibility to redistribute and reuse stored data. In some cases, valuable experimental data may be publicly available after the project end.

Reusage of deposited data is ensured by the policies of targeted repositories. The UBFC institutional repository Cherry is generated for long-term conservation without any time limitation. On the other hand, depositing research data in Chemotion is guaranteed until 2028, with official intents to prolong this period by additional contracts (<https://www.chemotion-repository.net/home/directive>).

2.4.3. Will the data produced in the project be useable by third parties, in particular after the end of the project?

Access to the generated project data will be enabled to third parties even after the project period. As previously stated, Cherry enables data conservation with no time limitations, while Chemotion strives to do so as well.

2.4.4. Will the provenance of the data be thoroughly documented using the appropriate standards?

The appropriate standard for data provenance will be utilized among Consortium representatives. Once the first data is conserved in both repositories, it will be more clear which standard for data provenance is the most suitable to be documented.

2.4.5. Describe all relevant data quality assurance processes. Further to the FAIR principles, DMPs should also address research outputs other than data, and should carefully consider aspects related to the allocation of resources, data security and ethical aspects.

MET-EFFECT will strive to follow the best practices for ensuring data quality by:

- checking and monitoring data, cleansing activities that will consequently lead to enhanced data quality
- updating data that leads to more accuracy
- ensuring data consistency and accuracy using e.g. data filtering

By following these steps, the project will focus on avoiding mistakes such as inaccurate data, duplicated or hidden data, or ambiguous data.

3. Other research outputs

In addition to the management of data, beneficiaries should also consider and plan for the management of other research outputs that may be generated or re-used throughout their projects. Such outputs can be either digital (e.g. software, workflows, protocols, models, etc.) or physical (e.g. new materials, antibodies, reagents, samples, etc.). Beneficiaries should consider which of the questions pertaining to FAIR data above, can apply to the management of other research outputs, and should strive to provide sufficient detail on how their research outputs will be managed and shared, or made available for re-use, in line with the FAIR principles.

As proposed, MET-EFFECT will develop protocols for metal recycling as well as for some recycling chemicals (e.g. acetone). These protocols will be primarily documented in the form of hard copy and afterwards transferred to the corresponding digital form.

4. Allocation of resources

4.1. What will the costs be for making data or other research outputs FAIR in your project (e.g. direct and indirect costs related to storage, archiving, re-use, security, etc.)?



At this stage of the project implementation, no costs are foreseen for open experimental results. The use of both identified repositories (Chemotion or Cherry) is free of charge, and the data are provided and licensed as Open Data. In case of unpredicted costs, DMP versions will be updated.

4.2. How will these be covered? Note that costs related to research data/output management are eligible as part of the Horizon Europe grant (if compliant with the Grant Agreement conditions).

The planned costs for Open Access publications and data management workspace in a project website will be allocated to the Category B of the project budget. In Chemotion, the data size per user is limited to 10 GB. On the other hand, any other unforeseen costs linked to data management may be reimbursed during the project duration and under the conditions defined in the Grant Agreement.

4.3. Who will be responsible for data management in your project?

The strict implementation of the Data Management Plan will require proper coordination and monitoring at the level of work packages and the overall project. Thus, Consortium representatives are nominated as responsible persons for data management:

Nominated person	Institution	Contact
Ljiljana Mihajlović-Lalić	ICFCB	ljiljanam@chem.bg.ac.rs
Stefan Nikolić	ICFCB	snikolic@chem.bg.ac.rs
Maria João G. Ferreira	IST-ID	m.joao.ferreira@tecnico.ulisboa.pt
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Hristina Hristova	VRLS	office@venusroses-labsolutions.eu
Monica Trif	CENTIV	mt@centiv.de

Nominated team members will comply with personal data protection rules (Regulation EC 45/2001).

The national repository, Cherry, is entitled to:

- define a list of data users who will have usage rights to access, upload, edit, and download data
- perform initial setup of the hardware and software tools
- enable creating the project workspace in the repository
- maintain hardware and software necessary for data conservation
- follow regular security assessments after the initial evaluation.

In the case of force majeure, UBFC will not be responsible for inadequate data conservation.

Regarding the conservation of metadata in Chemotion, the project collection will start in the following three months. Thus, the updated version of the Data Management Plan will report this activity.

4.4. How will long term preservation be ensured? Discuss the necessary resources to accomplish this (costs and potential value, who decides and how, what data will be kept and for how long).

The national repository Cherry is established for long-term data conservation and is not time-limited. Moreover, the project website will be active for at least two years after the project's official ending. This activity aims to disseminate research data further to the targeted public (company representatives, policymakers, general public).

5. Data security

5.1. What provisions are or will be in place for data security (including data recovery as well as secure storage/archiving and transfer of sensitive data)?

Consortium representatives will act according to a well-defined policy for data security that will comprehend project participants. At this project stage, it is not foreseen to generate, collect or store any kind of sensitive data. Thus, no specific regulations regarding this matter will not be defined.

The national research data infrastructure is hosted at the RCUB University of Belgrade Computer Centre, which is entitled to data maintenance and backup (<https://rcub.bg.ac.rs/en/>). The research data platform, Chemotion is hosted at the Karlsruhe Institute of Technology (KIT). The corresponding directive to use the service of Chemotion is given at <https://www.chemotion-repository.net/home/directive>.

5.2. Will the data be safely stored in trusted repositories for long term preservation and curation?

Open results in Chemotion will be safely stored for long time conservation. As the project implementation continues, it is foreseen to generate valuable data for e.g. patent draft, which will be retained. Storing research data in Chemotion is guaranteed until 2028, with the official intent to prolong this period by additional contracts (<https://www.chemotion-repository.net/home/directive>).

6. Ethics

6.1. Are there, or could there be, any ethics or legal issues that can have an impact on data sharing? These can also be discussed in the context of the ethics review. If relevant, include references to ethics deliverables and ethics chapter in the Description of the Action (DoA).

At this project stage, all identified ethical parameters are documented in the recently submitted Deliverable Report D8.1. OEI - Requirement No. 1. Thus, the nominated Ethics Advisor and internal Ethics Committee will be responsible for ethics regulations linked to data management. In parallel with this action, the project participant will follow EU, national, and international regulations regarding data storage alongside principles of research integrity.



6.2. Will informed consent for data sharing and long term preservation be included in questionnaires dealing with personal data?

Uploading data with personal information to any project repository will be possible only based on ethics approvals. In that sense, the generated data will be unidentified, meaning that e.g. low-resolution identifying variables such as gender or age can be stored while all others (name, phone number, address, e-mail, national ID number) will be kept as confidential data.

7. Other issues

Do you, or will you, make use of other national/funder/sectorial/departmental procedures for data management? If yes, which ones (please list and briefly describe them)?

As previously stated, MET-EFFECT implementation will be in accordance with all relevant institutions, in the first place, European Commission policy and, further, institutional policies and regulations linked to data management. For successful action in this domain, participants will be encouraged to use MareData recommendations for data management (<https://digital.csic.es/bitstream/10261/173801/2/Maredata-recommendations-ENG.pdf>).

