

---

## DMP du projet "Mychem Software Management Plan"

Plan de gestion de données créé à l'aide de DMP OPIDoR, basé sur le modèle "Research Software Management Plan template (PRESOFT project)" fourni par PRESOFT projet.

### Plan Details

<b>Plan title</b>	DMP du projet "Mychem Software Management Plan"
<b>Language</b>	fra
<b>Creation date</b>	2020-04-02
<b>Last modification date</b>	2021-09-14
<b>Identifiant</b>	5940

### Project Details

**Project title** Mychem Software Management Plan

#### Abstract

#### Research outputs :

1. Mychem (Logiciel)

### Contributors

Name	Affiliation	Roles
Jérôme Pansanel - <a href="https://orcid.org/0000-0002-7067-5009">https://orcid.org/0000-0002-7067-5009</a>		<ul style="list-style-type: none"><li>• Coordinateur du projet</li><li>• Personne contact pour les données</li><li>• Responsable du plan</li></ul>

#### Droits d'auteur :

Le(s) créateur(s) de ce plan accepte(nt) que tout ou partie de texte de ce plan soit réutilisé et personnalisé si nécessaire pour un autre plan. Vous n'avez pas besoin de citer le(s) créateur(s) en tant que source. L'utilisation de toute partie de texte de ce plan n'implique pas que le(s) créateur(s) soutien(nen)t ou aient une quelconque relation avec votre projet ou votre soumission.

# DMP du projet "Mychem Software Management Plan"

---

## 1. Metadata

**Software name** - *If you need to choose a name, avoid the name of a brand and other software names*

Mychem

---

**Short description of the software** - *A short sentence describing your software*

The Mychem software is an extension for MySQL and MariaDB. It aims to provide functions for converting chemical data and computing chemical properties.

---

**Software web page or website**

<https://mychem.github.io>

---

**Link to source code or package**

<https://github.com/mychem/mychem-code>

---

**Contact (email adress)**

jerome.pansanel@iphc.cnrs.fr

---

**Research unit in charge of the software**

Instittut Pluridisciplinaire Hubert Curien

---

**Main developers and their affiliations**

- Jérôme Pansanel (CNRS)
  - Aurélie De Luca
  - Bjoern Gruening (University of Freiburg)
- 

**Software version**

Version 1.0.1

---

#### Date of the software version

2021-02-23

---

#### Licence

*GPL v2 license*

---

Scientific discipline - *For example according to the ERC*  
[https://erc.europa.eu/sites/default/files/document/file/ERC\\_Panel\\_structure\\_2018.pdf](https://erc.europa.eu/sites/default/files/document/file/ERC_Panel_structure_2018.pdf) or to the EGI scientific classification: [https://wiki.eqi.eu/wiki/Scientific\\_Disciplines](https://wiki.eqi.eu/wiki/Scientific_Disciplines)

Data management and computational chemistry

---

#### Main functionalities - *In the form of keywords*

**Chemical data conversion, chemical property computation, substructure search, fingerprint management.**

---

#### Main technical characteristics - *In the form of keywords*

MySQL User-Defined Functions, OpenBabel, C and C++ languages, CMake

---

#### Other keywords

Question sans réponse.

---

## 2.1 Software context: History

#### Preparatory material - *Identify and date the preparatory material*

Question sans réponse.

---

Specifications (if any), conception model (UML or other), use cases... - *References and dates for the specifications,*

*conception model...*

Question sans réponse.

---

**Previous software versions - *Identify and date the previous versions***

See <https://raw.githubusercontent.com/mychem/mychem-code/master/NEWS>

---

**Components included in the software and external dependencies - *Identify and describe the different components that are part of the software: name, version, date, authors, website, licence...***

The software requires MySQL (or MariaDB) and OpenBabel.

---

**New components to be included in the new version of the software - *Identify and describe the different components***

The next planned enhancement are:

- using a continuous integration platform for testing purposes ;
  - supporting the last version of OpenBabel
- 

**Roadmap (*Link*)**

Question sans réponse.

---

**Are there other software developments with similar functionalities? Which are the differences?**

Some software with similar functionalities is available. The main differences are:

- the software is working with another types of database system (PostgreSQL or Oracle) ;
  - it is closed-source and proprietary software
- 

**Publications, data and other associated productions - *For example: the team publications to explain the software design or to show the obtained scientific results by using the software***

Question sans réponse.

---

Up to this date (to be given), estimation of the software's cost - *Number of person/months for example*

Over the year 2019, the development of the Mychem software as required 6 days of work for a single engineer.

---

## 2.2 Software context: Project(s) related to the software

### Project(s) related to the software

	Project 1	Project 2
Project's name ( <i>The project's name may be different from the software's name</i> )	This software is mainly developed by Jerome Pansanel as part of his work at IPHC. It is not related to a specific project.	
Type of the project ( <i>ANR, H2020...</i> )		
Identifier of the project		
Start date of the project ( <i>YYYY-MM-DD</i> )		
End date of the project ( <i>YYYY-MM-DD</i> )		
Project web site		
Framework in which the software is developed*		
Allocated resources and funding ( <i>human, financial, hardware</i> )		
Possible constraints linked to the project**		
Partners and role in relation to the software		
Is the software a deliverable of the project?		

\*Framework in which the software is developed: for example, the software may be the objective of the project or may be developed in a work package. Previous developments must be declared in the grant agreement or consortium agreement. Define the new developments in this project.

\*\*Possible constraints linked to the project: for example mandatory licence for the project developments in the grant agreement or in the consortium agreement.

---

## 2.3 Software context: Legal issues and distribution policy

**Intellectual property - Identify authors, rightholders.**  
*In the framework of a project the intellectual property is part of the consortium agreement.*

CNRS and University of Strasbourg hold the intellectual property.

---

### Rightholders or copyright statement

Copyright (C) 2009-2021 by CNRS and University of Strasbourg.

---

**Distribution policy - Constraints linked to the project (s), the partners and their organisms**

It is a free and open-source software. There are no constraints.

---

**Licence(s) - Beware of possible heritage and licence compatibility issues. Mention the licences of the documentation, of the web site...**

*GPL v2 license and BSD for the documentation.*

---

**If the code is to be open, when will it be open? - To be validated with the possible partners and according to the constraints linked to the funding**

Question sans réponse.

---

**Management of the intellectual property of external contributions - Rights' transfer agreement to be planned**

Question sans réponse.

---

**Non disclosure or privacy clauses and sensitive data processing (if needed)**

Question sans réponse.

---

### **3.1 Software features: Scientific goals**

**Objectives, expected results - Describe in a synthetic way the scientific goals and the expected results linked to the software**

Question sans réponse.

---

### **3.2 Software features: Usage and distribution objectives**

**Planned or considered lifespan**

Question sans réponse.

---

**Planned usage - *What for (publications, teaching, production level usage, industry level usage)?***

This software aims to provide functions for the MySQL and MariaDB relational database management system, to facilitate the development of portals and tools for the management of chemical data.

---

**Target public - *For example: researchers, team, restricted distribution, collaboration, wide distribution...***

The software intends to be used by researchers and engineers who are dealing with chemical data. It can also be used during training, for example when working on binary molecular fingerprints.

---

**Planned user support - *Type of support, tools, resources, quality of service for the users. For example, user support, ticket system, a person in "best effort"...***

The support is provided through:

- a complete on-line documentation;
- a ticket system;
- a developer (*best effort mode*).

---

**Distribution goals - *The software is "for internal use only", the software will be published via an article, the software will be distributed widely...***

The software is freely available on GitHub.

---

**Collaboration community wished - *If yes, which one?***

- Yes
- Yes

We are looking for developers and testers.

---

**Adequacy of the resources (development, maintenance...) to the distribution goals - *Are the available resources suitable? (human, financial and material resources)***

Human resources are enough for the maintenance of the software, however additional competences would be welcome for specific developments.

---

**Risk analysis - *A risk analysis may be useful before launching an expensive development or an unwise distribution***

No risk analysis has been done so far.

---

**Software preservation - *What is the objective for the preservation and what is the solution used? - Please distinguish short term backup and long term archiving***

The source code is saved on several sites with version control system. Backup from stable versions are performed on the laboratory storage server. The code is also correctly indexed by the Software Heritage project:

<https://archive.softwareheritage.org/swh:1:dir:8e7c56ee116ce2797ab0152c88136a71dc9a13f9;origin=https://github.com/mychem/mychem-code/>

---

### 3.3 Software features: Technical features

#### Used technologies

C, C++, CMake

---

**Dependencies** - *OS, SDK, libraries, browser, external APIs...*

Mychem depends on MySQL (or MariaDB) development libraries and OpenBabel libraries.

---

**Already existing components reuse** - *Technical constraints*

Two files (c++ source code) of the [OpenBabel project](#) are used.

---

**Documentation** - *Give the documentation's url*

The documentation is available on the following Websites:

- <https://mychem.github.io/docs/> (online)
  - <https://github.com/mychem/mychem-documentation> (source code)
- 

**Used norms and standards** - *Example: ISO norm of the development language*

Question sans réponse.

---

## 4. Team organisation

**Governance** - *For example the organisation officially in charge of the software, a consortium...*

IPHC is the the organisation officially in charge of the software.

---

**Consortium agreement including governance, development and future of the software** - *In the case of a shared development between several organisms - If the software is developed in the framework of a project, the consortium agreement must take it into account.*

Question sans réponse.

---

**Team** - *List the members of the team. Indicate for each person its status (employee /institution, internship, student, retired...) and their participation dates*

Jérôme Pansanel (CNRS)

---

**Organisation around the software** - *Responsibilities of the different actors: development, training, support, distribution, translation... - Distinguish the different roles: leader, main developers, minor contributors, scientific contributors (no code writing), documentation writers...*

Question sans réponse.

---

**Costs and funding distribution**

Question sans réponse.

---

**Type of development** - *Collaborative or not (practical organisation of the collaboration). Note that the 5th section details the development organisation*

Collaborative development.

---

**Actions to be planned in case of a person's leave**

Question sans réponse.

---

## 5. Development organisation

**Development team** - *On one or several sites, depending on one or several institutions...*

The team is distributed on several sites.

---

**Development plan** - *Roadmap including the new versions, functionalities planned and dates.*

Question sans réponse.

---

**Development methods, used standards, tools and infrastructures (code repository)** - *Example: tools for version management and collaborative development*

Question sans réponse.

---

**Actor's responsibilities in the development**

Question sans réponse.

---

**Quality procedures** - *For example, actions taken to foster the software maintainability, best practices applied, verification tests...*

The software integrates a test suite. A new version of Mychem is released only if all tests are executed successfully.

---

**Security (taken into account in the development)**

Question sans réponse.

---

**Version delivery, bugs, tests and validation management** - *Are there testing or other validation procedures? With which follow-up? Are they to be given to final users? How do you manage bugs?*

Question sans réponse.

---

**Documentation production management (internal and for users, installation and requirements, use examples)** - Explain how the documentation is produced and updated for each version (responsibilities, organisation...)

Question sans réponse.

---

**Describe main planned evolutions** - For example: integration in other projects, software translations...

Question sans réponse.

---

**If external participations are expected and possible, which are the rules (validation of the contributions, contribution integration in the major versions, participation integration)?** - It is advisable to define accurately the rules before any external participation.

Question sans réponse.

---

## 6. Distribution organisation

**Reference repository** - For example: the link to the software version on SourceSup, Zenodo or Gitlab IN2P3

<https://github.com/mychem/mychem-code>

---

**Persistent identifier** - Indicate for example the DOI of your software

Question sans réponse.

---

**Citation form** - You can suggest to cite the publication that describes your software or the one that seems to be the most important.

Otherwise you may propose for example: "author(s), software name, short description, version, date, url"

J. Pansanel, A. De Luca and B. Gruening. Mychem. *Version. Date.* <https://github.com/mychem/mychem-code>

---

**Links to articles or other research outputs external to the team and that use the software** - *Important: to show that the software is used outside the development team or the original laboratories.*

- Schmidt U, Struck S, Gruening B, Hossbach J, Jaeger IS, Parol R, Lindequist U, Teuscher E, Preissner R. SuperToxic: a comprehensive database of toxic compounds. *Nucleic Acids Res.* 2009 Jan;37 D295-9. doi:10.1093/nar/gkn850. PMID: 19004875; PMCID: PMC2686515.
  - J.-L. Faulon and A. Bender "Handbook of Chemoinformatics Algorithms". CRC Press, 2010.
  - Pirhadi S, Sunseri J, Koes DR. Open source molecular modeling. *J Mol Graph Model.* 2016;69:127-143. doi:10.1016/j.jmkgm.2016.07.008
- 

**Referencing (announces, websites of the scientific community...)**

[https://openbabel.org/wiki/Related\\_Projects](https://openbabel.org/wiki/Related_Projects)

---

**Communications** - *Conferences, posters, flyers...*

Question sans réponse.

---

**Publications in a software journal**

Question sans réponse.

---

**User support (such as offered to the users)**

Ticket management system proposed by GitHub:

<https://github.com/mychem/mychem-code/issues>

---

**Usage indicators** - *Number of downloads, number of exchanges with users...*

Question sans réponse.

---

## 7. SMP management

## Person in charge of this SMP

Jérôme Pansanel

---

## Is the SMP required by a project funding, an agreement, contract or other?

The SMP is not required by anyone.

---

**Organisation to write and update the SMP and monitor actions and goals** - *Is there a collaborative place for this SMP? Is it a text document? What is the update frequency or it is updated continuously? What type of events triggers an update? Who are the actors?*

*The current document has been created with the DMP OPIDoR service. Please don't forget to keep the successive versions in your local workspace.*

This document is hosted on DPM OPIDiR. It will be updated in the following case:

- new version of the software ;
  - new related projects ;
  - new publications.
- 

## Distribution of this SMP

- Public
  - Public
- 

**Links with the current project's Data Management Plan (if any)** - *If yes, is there a reference model or important points to develop? Is this SMP a part of the project's DMP? - In certain calls, the DMP template includes a section for software, but a DMP is focused on data, not on software and it is not designed for software management.*

This project is not linked with a DMP.