

---

# 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

### Produits de recherche :

1. Mychem (Logiciel)

## Contributeurs

Nom	Affiliation	Rôles
Jérôme Pansanel		<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

Mychem

---

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

---

<https://mychem.github.io>

---

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

---

jerome.pansanel@iphc.cnrs.fr

---

Instititut Pluridisciplinaire Hubert Curien

---

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

Version 1.0.1

---

2021-02-23

---

*GPL v2 license*

---

Data management and computational chemistry

---

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

---

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

---

Question sans réponse.

---

## 2.1 Software context: History

Question sans réponse.

---

Question sans réponse.

---

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

---

The software requires MySQL (or MariaDB) and OpenBabel.

---

The next planned enhancement are:

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

Question sans réponse.

---

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
- 

Question sans réponse.

---

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 1

Project  
2

Project's name (*The project's name may be different from the software's name*)

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 (*ANR, H2020...*)

Identifier of the project

Start date of the project (*YYYY-MM-DD*)

End date of the project (*YYYY-MM-DD*)

Project web site

Framework in which the software is developed\*

Allocated resources and funding  
(*human, financial, hardware*)

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

CNRS and University of Strasbourg hold the intellectual property.

---

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

---

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

---

*GPL v2 license and BSD for the documentation.*

---

Question sans réponse.

---

Question sans réponse.

---

Question sans réponse.

---

### 3.1 Software features: Scientific goals

Question sans réponse.

---

### 3.2 Software features: Usage and distribution objectives

Question sans réponse.

---

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.

---

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.

---

The support is provided through:

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

The software is freely available on GitHub.

---

- Yes

We are looking for developers and testers.

---

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

---

No risk analysis has been done so far.

---

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

C, C++, CMake

---

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

---

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

---

The documentation is available on the following Websites:

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

---

Question sans réponse.

---

## 4. Team organisation

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

---

Question sans réponse.

---

Jérôme Pansanel (CNRS)

---

Question sans réponse.

---

Question sans réponse.

---

Collaborative development.

---

Question sans réponse.

---

## 5. Development organisation

The team is distributed on several sites.

---

Question sans réponse.

---

Question sans réponse.

---

Question sans réponse.

---

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

---

Question sans réponse.

---

Question sans réponse.

---

Question sans réponse.

---

Question sans réponse.

---

Question sans réponse.

---

## 6. Distribution organisation

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

---

Question sans réponse.

---

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

---

- 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.jmgl.2016.07.008
- 

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

---

Question sans réponse.

---

Question sans réponse.

---

Ticket management system proposed by GitHub:

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

---

Question sans réponse.

---

## 7. SMP management



Jérôme Pansanel

---

The SMP is not required by anyone.

---

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.
- 

- Public
- 

This project is not linked with a DMP.