
Mychem Software Management Plan

Plan de gestion de données créé à l'aide de DMP OPIDoR

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Modèle du PGD : Research Software Management Plan template (PRESOFT project)

Dernière modification du PGD : 14/09/2021

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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>

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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 (<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

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>

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- J.-L. Faulon and A. Bender "Handbook of Chemoinformatics Algorithms". CRC Press, 2010.
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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.

