

# ChemPharos: a comprehensive database of plastic-degrading enzymes, powered by Enalos Tools

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## 1. Introduction

The use of plastics, in everyday life, has contributed significantly to environmental pollution. In response to the escalating issue of plastic waste, natural degradation methods have emerged as potential waste management protocols. Notably, biodegradation by microorganisms has gained prominence as a preferred approach among environmentally conscious societies [1]. To address this environmental issue, we present ChemPharos, a database tailored for modelling-reading chemical datasets powered by the Enalos Cloud Platform [2] and demonstrate its use for rapid prediction of plastic degrading enzymes.

ChemPharos is a computational framework designed to store various data regarding chemicals, their properties and their functionalities, illustrated here via a dataset of enzymes that can degrade plastic polymers. The scope of the specific modelling-ready dataset is to harness cutting-edge Artificial Intelligence (AI) and Machine Learning (ML) tools for Micro and Nano-Plastics (MnNP) risk assessment as part of the EU-funded Marie Curie Training Network, Plastic Underground. The ultimate goal of the Plastic Underground instance of ChemPharos is to serve as a robust platform facilitating the seamless integration and automation of Molecular Dynamics (MD) simulations, enabling in-depth investigations into the impact of MnNP in soil and groundwater environments.

One of the key objectives of Plastic Underground is to fundamentally reshape MnNP risk assessment methodologies by integrating a comprehensive cloud-based platform with advanced data analytics and simulation functionalities. The deployment of ChemPharos aims to catalyse understanding of methods for remediation of plastic pollution in terrestrial and subterranean aquatic ecosystems. This platform is specifically designed to yield innovative insights into the behavioural dynamics of MnNPs and their subsequent environmental ramifications, thereby augmenting current strategies in environmental sustainability management.

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## 2. Data Collection

MySQL was selected as the Relational Database Management System (RDBMS) for ChemPharos due its known fast performance, scalability, reliability, and robust security features. MySQL, being open source, offers cost-effective management of large datasets and facilitates seamless integration with server-side java scripting [3]. Moreover, its compatibility with cloud environments ensures seamless integration for deployment and scaling within the cloud infrastructure. Additionally, MySQL provides tools for administration, monitoring, and optimization, aiding in efficient database management and performance monitoring [4].

Integrating data from ChEMBL, an existing open-source bioactivity database that is regularly updated [5], enriches ChemPharos by providing valuable insights for Micro and Nano Plastic (MnNP) risk assessment. By integrating ChEMBL into ChemPharos, the Plastic Underground project aims to enhance automated molecular simulations and enable explicit data insertion and modification with well-defined authorization mechanisms.

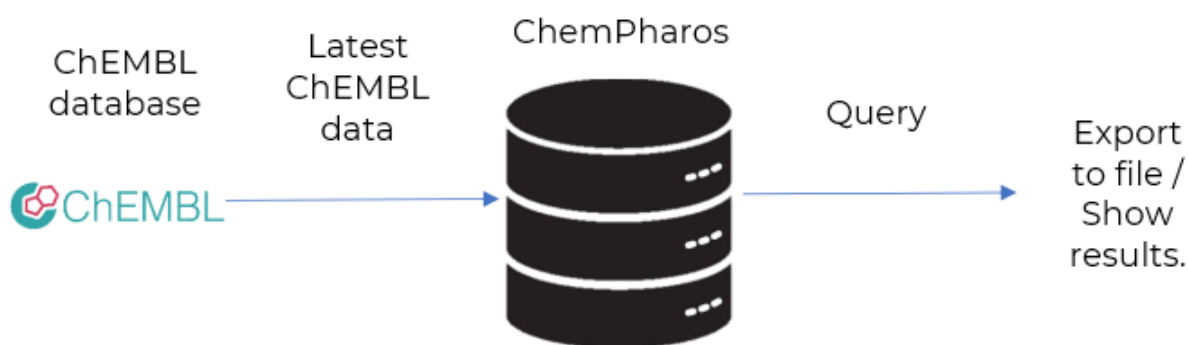


Figure 1: Proposed data workflow of ChEMBL and ChemPharos.

## 3. Tools

Java (<https://www.java.com/en/>) has been chosen as the backend server-side programming language of ChemPharos for its versatility, portability and robust ecosystem [6].

Javascript (<https://www.javascript.com/>) is used as the scripting language for visualisations, empowering the user interface with dynamic and interactive content. [7].

ZK Framework (<https://www.zkoss.org/product/zk>) and the ZK User Interface Markup Language (ZUL) has been selected for developing the front end due to its component-based architecture which facilitates modular development of the graphical user interface [8].

Keycloak (<https://www.keycloak.org/>) has been employed as the Identity and Access Management System for ChemPharos to ensure that only authorised individuals (curators) have access to sensitive data and functionalities. [9].

Wildfly (<https://www.wildfly.org/>) has been selected as the runtime server for deploying and running the Java based backend of ChemPharos.

## 4. User Interface (UI)

Figures 2 and 3 provide a snapshot of the user interface, and how the user selects the features of interest.

### 4.1 Search Configuration

Advanced Search Configuration Set Output Configuration

compound\_records  
 target\_dictionary  
 tissue\_dictionary

Logical Operator: AND Table Attributes: tissue\_id

Unique Values  Inequality

Excluded

Filter Excluded

- 2
- 4
- 7
- 9
- 14
- 23
- 25

Included

Filter Included

- 6
- 7
- 9
- 14

drug\_record\_id  
substrate\_record\_id  
metabolite\_record\_id  
pathway\_id  
pathway\_key  
enzyme\_name  
enzyme\_id  
met\_conversion  
organism  
tax\_id  
met\_comment

record\_id  
molregno  
warning\_type  
warning\_class  
warning\_description  
warning\_country  
warning\_year  
efo\_term  
efo\_id  
efo\_id\_for\_warning\_class

level1  
level2  
level3  
level4  
level5  
level1\_description  
level2\_description  
level3\_description  
level4\_description

compound\_records

record\_id  
molregno  
doc\_id  
compound\_key  
compound\_name  
src\_id  
src\_compound\_id  
cidx

drug\_indication

drugind\_id  
record\_id  
molregno  
max\_phase\_for\_ind  
mesh\_id  
mesh\_heading  
efo\_id  
efo\_term

hrac\_classification

hrac\_class\_id  
active\_ingredient  
level1  
level1\_description  
level2  
level2\_description  
level3  
hrac\_code

target\_dictionary

tid  
target\_type  
pref\_name  
tax\_id  
organism  
chembl\_id  
species\_group\_flag

tissue\_dictionary

tissue\_id  
uberon\_id  
pref\_name  
efo\_id  
chembl\_id  
bto\_id  
caloha\_id

chembl\_id\_lookup

chembl\_id  
entity\_type  
entity\_id  
status  
last\_active

indication\_refs

indref\_id  
drugind\_id  
ref\_type  
ref\_id

ligand\_eff

activity\_id  
bel  
sei  
le

mechanism\_refs

mecref\_id  
mec\_id  
ref\_type  
ref\_id

Figure 2: Advanced Search Configuration Page of ChemPharos.

Output Configuration

activities  
 molecule\_dictionary  
 assays

Excluded

Filter Excluded

- max\_phase
- therapeutic\_flag
- dosed\_ingredient
- structure\_type
- chebi\_par\_id
- molecule\_type
- first\_approval

Included

Filter Included

- molregno
- pref\_name
- chembl\_id

Set
Cancel

activities

activity\_id  
assay\_id  
doc\_id  
record\_id  
molregno  
standard\_relation  
standard\_value  
standard\_units  
standard\_flag  
standard\_type  
activity\_comment  
data\_validity\_comment  
potential\_duplicate  
pchembl\_value  
bao\_endpoint  
uo\_units  
quid\_units  
toxi  
upper\_value  
standard\_upper\_value  
src\_id  
type  
relation  
value  
units  
text\_value  
standard\_text\_value  
action\_type

molecule\_dictionary

molregno  
pref\_name  
chembl\_id  
max\_phase  
therapeutic\_flag  
dosed\_ingredient  
structure\_type  
chebi\_par\_id  
molecule\_type  
first\_approval  
oral  
parenteral  
topical  
black\_box\_warning  
first\_in\_class  
chirality  
prodrug  
inorganic\_flag  
usan\_year  
availability\_type  
usan\_stem  
polymer\_flag  
usan\_substem  
usan\_stem\_definition  
indication\_class  
withdrawn\_flag  
chemical\_probe  
natural\_product

assays

assay\_id  
doc\_id  
description  
assay\_type  
assay\_test\_type  
assay\_category  
assay\_organism  
assay\_tax\_id  
assay\_strain  
assay\_issue  
assay\_cell\_type  
assay\_subcellular\_fraction  
tid  
relationship\_type  
confidence\_score  
curated\_by  
src\_id  
src\_assay\_id  
chembl\_id  
cell\_id  
bao\_format  
issue\_id  
variant\_id  
aidx

activity\_supp

as\_id  
rgid  
smid  
type  
relation

drug\_mechanism

mec\_id  
record\_id  
molregno  
mechanism\_of\_action  
tid

assay\_parameters

assay\_param\_id  
assay\_id  
type  
relation  
value

Figure 3: Output Configuration Page of ChemPharos.

## 5. Future Work

While ChemPharos is set for beta deployment on the Enalos Cloud Platform, upcoming enhancements are in the pipeline to elevate its capabilities, including:

- Optimisation of querying and export functionalities
- Paging of results

- AI and ML tools for MnNP risk assessments
- Automation of molecular dynamics simulations

These envisioned developments showcase ChemPharos' dedication to provide an adaptable, user-friendly platform that remains at the forefront of molecular data analysis and visualisation.

## 6. Conclusions

The ChemPharos platform provides an integrated and user-centric solution for molecular simulations and MnNP risk assessments. Fundamentally, the Plastic Underground instance of ChemPharos is designed not only to refine the process of MnNP risk evaluation but also to exemplify the progressive and collaborative ethos inherent in software development. This approach ensures that the platform remains adaptive and responsive, effectively addressing the dynamic needs and challenges faced by researchers and decision-makers in the scientific domain.

## 7. Acknowledgments

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