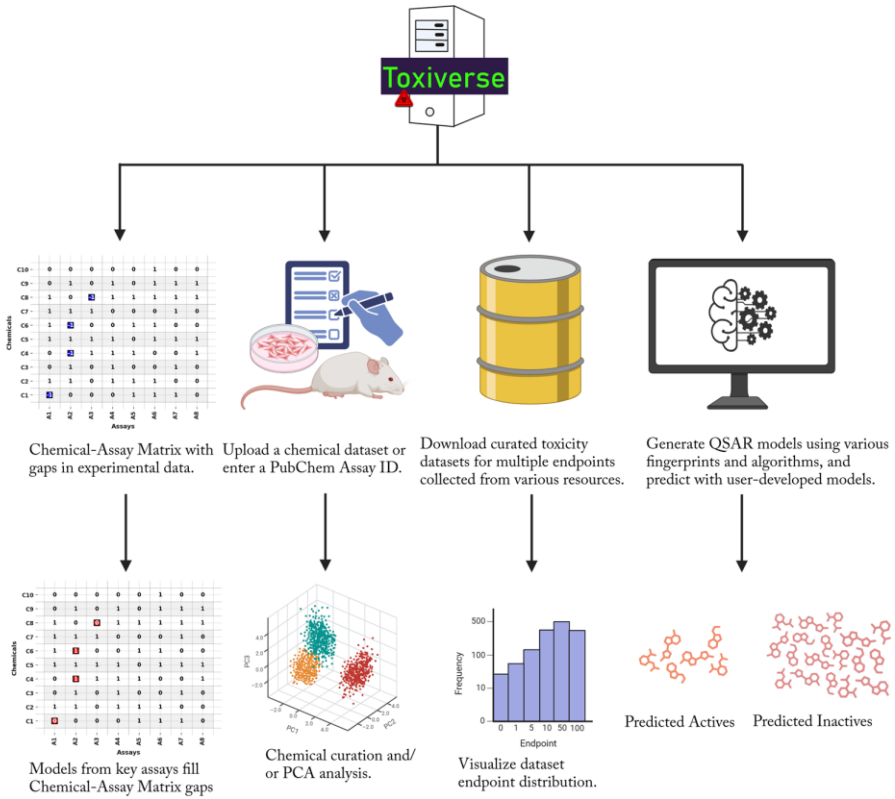
ToxiVerse

Tutorial

www.toxiverse.com

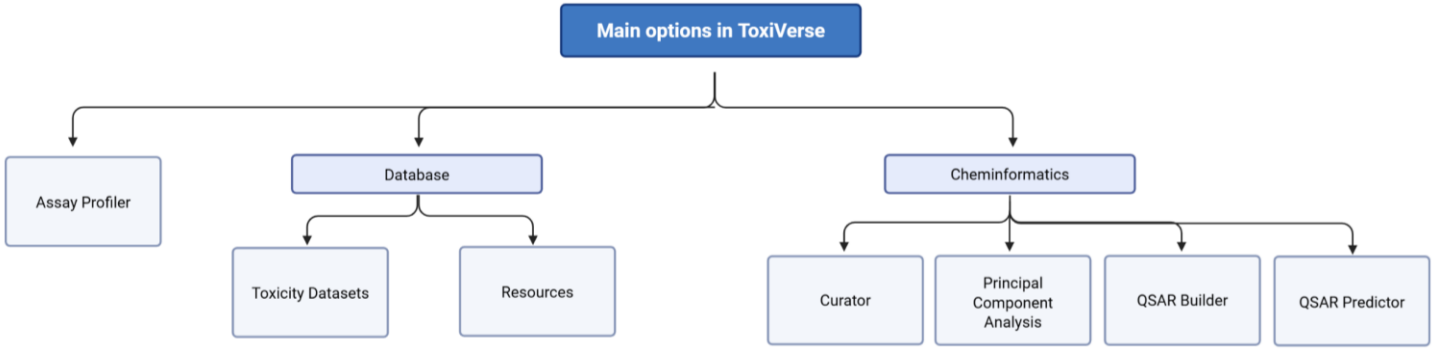


Contents

1. Introduction

Computational toxicology plays a significant role in identifying hazardous compounds to protect human health and the environment in a cost-effective manner. A major challenge in this field is the lack of publicly available and user-friendly computational tools that can be used for chemical risk assessment, especially by users with limited computational expertise.

To address this need, we developed Toxicology Universe (ToxiVerse), a web portal designed to assist toxicologists, pharmaceutical researchers, and chemists in assessing chemical safety. Please check Figure below for all the available options.



The options in ToxiVerse. They are explained in detail along with step-by-step tutorial in the following pages.

ToxiVerse offers the following functions:

I. **Profile bioassay results** from PubChem for chemicals of interest and fill experimental data gaps using QSAR models built from key assays.
II. **Download and visualize** curated toxicological datasets, including endpoint distribution plots. The integrated database includes over 26,000 chemicals across 43 toxicity endpoints, compiled from various sources.
III. **Create QSAR models** using either user-uploaded datasets or datasets retrieved from PubChem by providing an Assay ID. A variety of molecular descriptors and machine learning algorithms are supported.
IV. **Curate** and analyze datasets using **Principal Component Analysis** (PCA) before model development.
V. **Predict toxicity** for new chemicals using QSAR models developed within the platform.

1. These are the main modules.

ToxiVerse | Home | Assay Profiler | Database | Cheminformatics | Tutorial | Tasks | About

Welcome to

Database

- Toxicity Datasets
- Resources

2. Available options under the Database module.

ToxiVerse

Cheminformatics

- Upload or Retrieve Datasets
- Curator
- Principal Component Analysis
- QSAR Builder
- QSAR Predictor

3. Available options under the Cheminformatics module.

ToxiVerse is an online chemical data analysis portal that allows users to profile chemicals based on bioassay responses, download curated toxicological datasets, and perform common cheminformatics analyses. These include Quantitative Structure–Activity Relationship (QSAR) modeling, chemical space visualization, and more.

There are three main modules accessible from ToxiVerse. The Assay Profiler module enables users to profile chemicals based on their bioassay responses. The Database module provides access to curated toxicological datasets, along with detailed information about their data sources. The Cheminformatics module offers tools for visualizing chemical space and performing various cheminformatics analyses.

Assay Profiler

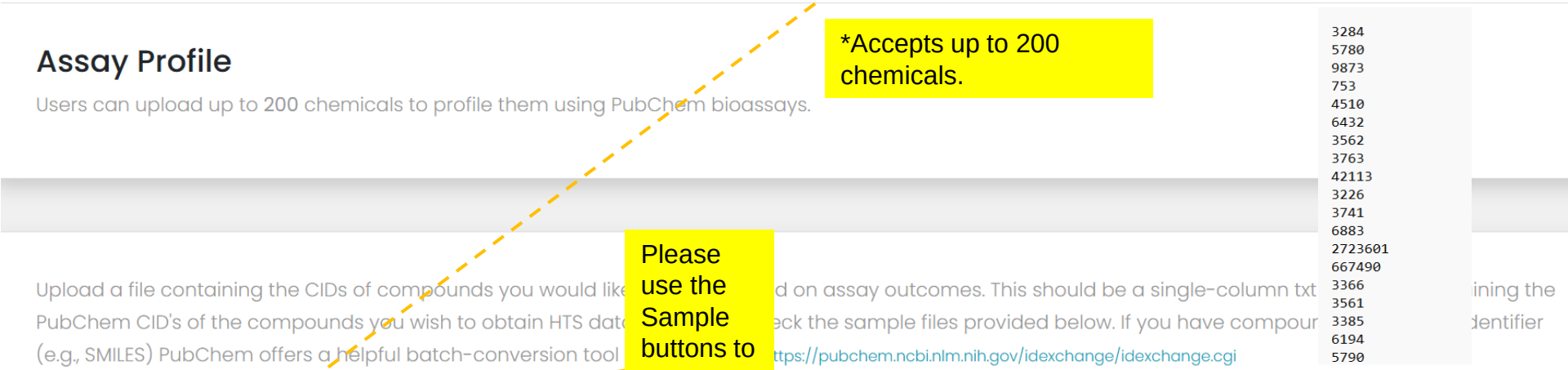
2. Assay Profiler

Users can upload up to 200 chemicals to profile them using PubChem bioassays. It fills experimental data gaps using QSAR models built from key assays.

1. Upload a file with PubChem Compound IDs eg: sample_dataset.txt

A sample file for Assay Profiler looks like below.

*Accepts up to 200 chemicals.



Please use the Sample buttons to download them.

Build Bioprofile

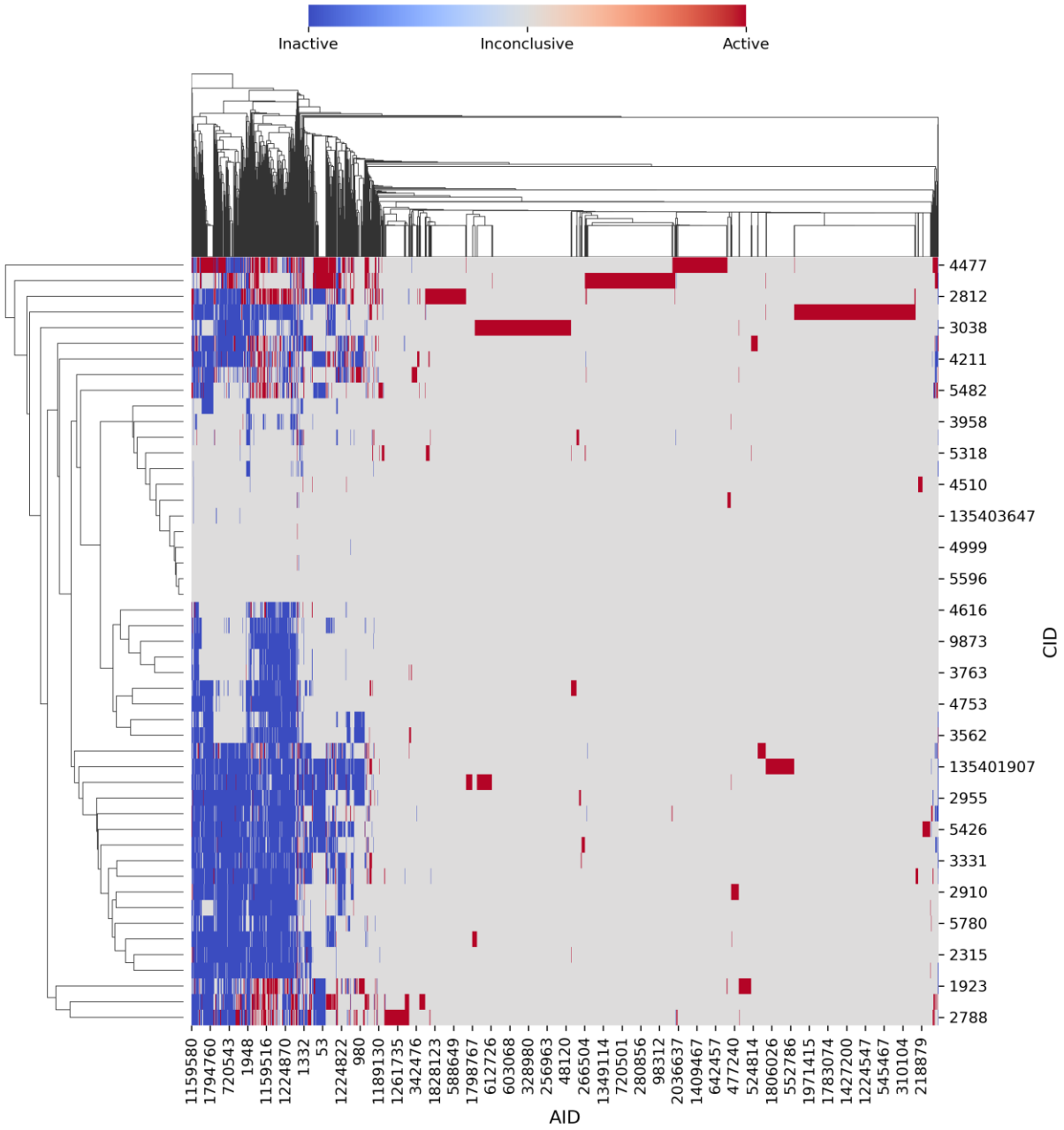
2. Click here

Results:

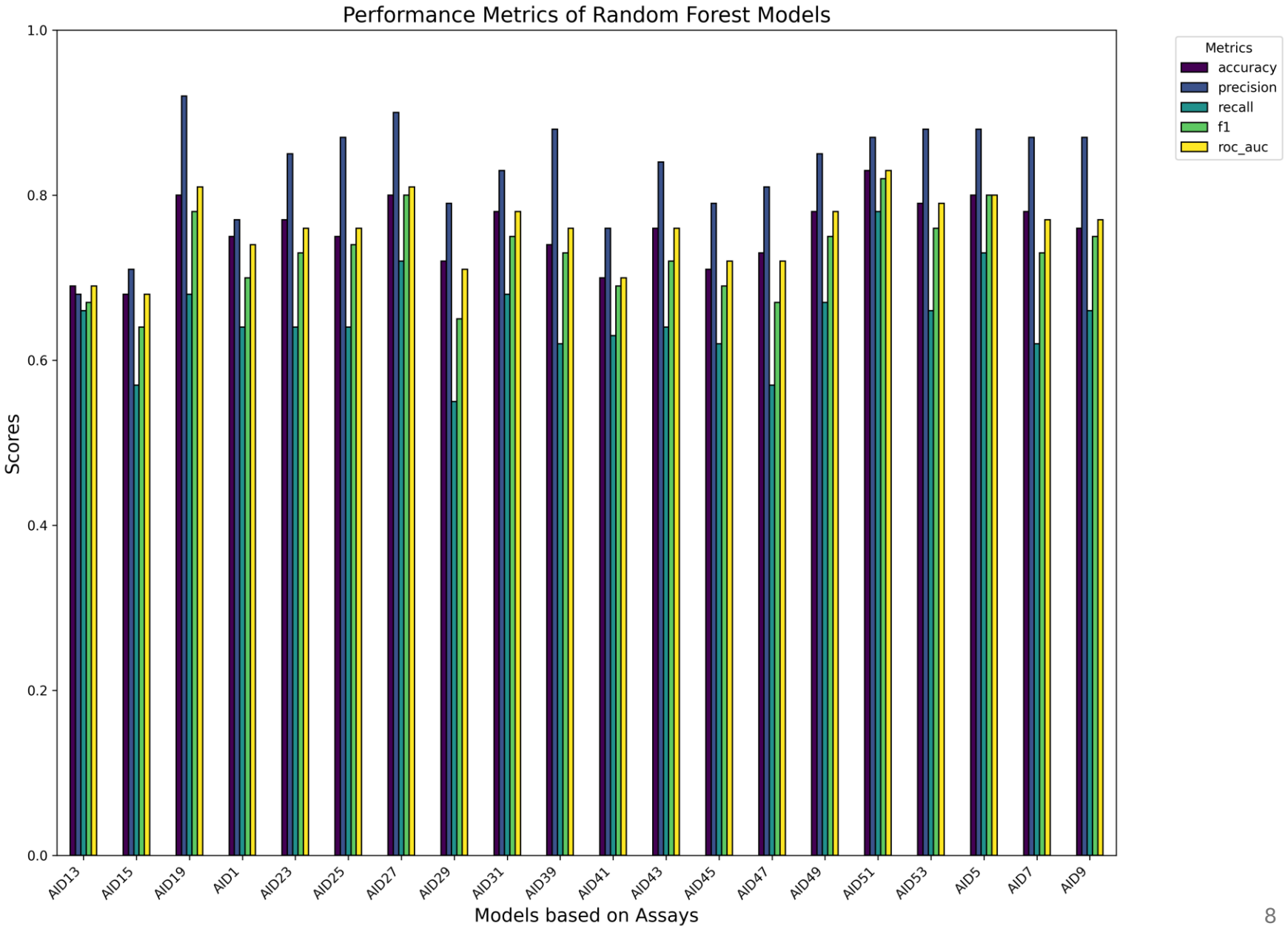
Download Bioprofile | Download Heatmap | Download Model Metrics | Download Model Metrics Plot | Download Filled Data Gaps Matrix

3. Click on options one by one to download the results.

Download heatmap result looks like this



Download Model Metrics Plot result looks like this



Download Bioprofile result looks like this

CID	1	7	9	19	25	29	67
4	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
11	-1	0	0	0	0	0	0
13	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0
33	0	-1	0	0	-1	0	0
34	0	0	0	0	0	0	0
51	0	0	0	0	0	0	0
66	0	0	-1	0	0	0	0
72	0	0	0	0	0	0	0
76	0	0	0	0	0	0	0
79	0	0	0	0	0	0	0

Download Model Metrics Plot looks like this

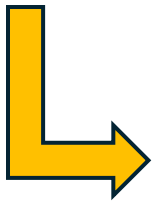
Model	accuracy	precision	recall	f1	roc_auc
AID1224834_rf_model	0.76	0.75	0.73	0.74	0.75
AID1224868_rf_model	0.77	0.83	0.75	0.79	0.77
AID743065_rf_model	0.73	0.75	0.7	0.73	0.73
AID743084_rf_model	0.75	0.81	0.69	0.75	0.75
AID743194_rf_model	0.85	0.96	0.76	0.85	0.86

Download Filled Data Gaps Matrix result looks like this

CID	1	7	9	19	25	29	67
4	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
11	1	0	0	0	0	0	0
13	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0
33	0	0	0	0	1	0	0
34	0	0	0	0	0	0	0
51	0	0	0	0	0	0	0
66	0	0	0	0	0	0	0
72	0	0	0	0	0	0	0
76	0	0	0	0	0	0	0
79	0	0	0	0	0	0	0

Please compare the top and bottom Tables. The CIDs (chemicals) and columns (AIDs) are shown. The above circled -1 values (blue circled) are replaced with 1s or 0s below (red circled) based on prediction scores.

Database



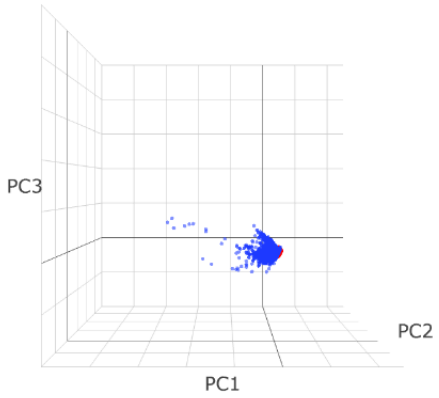
Toxicity Datasets

3. Toxicity Datasets

Allows users to download and visualize curated toxicological datasets, including endpoint distributions, and provides relevant bioassays for the selected endpoints. The dataset contains over 40,000 records for 26,000 chemicals across 43 endpoints, collected from various sources.

Select an endpoint in a toxicity dataset

Principal Component Analysis

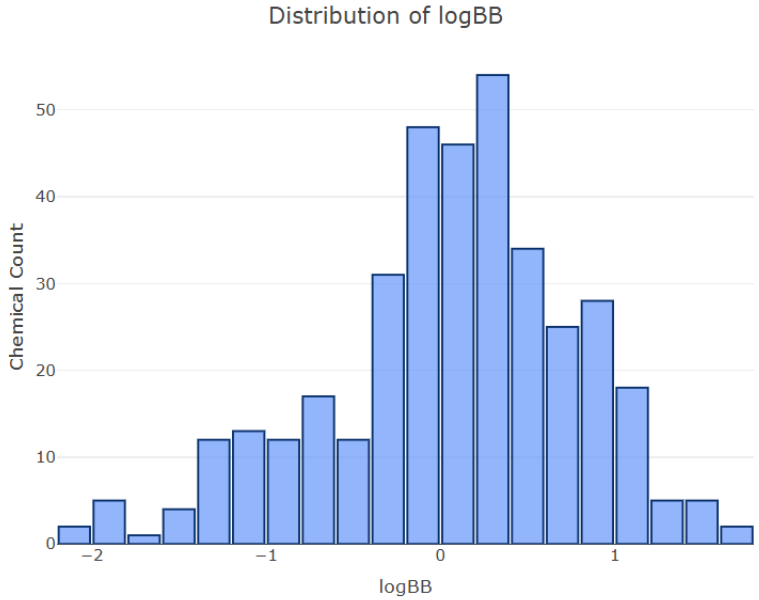


- Compounds with endpoint data in this dataset
- Compounds without endpoint data in this dataset
- Compounds from other datasets

Endpoint Distribution

Select endpoint:

logBB (BBB_curated)



Relevant bioassays

This is relevant Bioassays to the selected endpoint.

This is the table of bioassays ranked by their active rates (active compounds numbers in all bioassays).

Show 10 entries Search:

AID	Bioassay name	Inactive	Inconclusive	Active	Active rate
625256	DRUGMATRIX: Dopamine Transporter radioligand binding (ligand: [125I] RTI-55)	0	644	49	1
678713	Inhibition of human CYP2C9 assessed as ratio of IC50 in absence of NADPH to IC50 for presence of NADPH using 7-methoxy-4-trifluoromethylcoumarin-3-acetic acid as substrate after 30 mins	0	142	206	1
625204	DRUGMATRIX: Adrenergic beta1 radioligand binding (ligand: [125I] Cyanopindolol)	0	640	53	1
625205	DRUGMATRIX: Adrenergic beta2 radioligand binding (ligand: [3H] CGP-12177)	0	637	56	1
625207	DRUGMATRIX: Norepinephrine Transporter radioligand binding (ligand: [125I] RTI-55)	0	576	117	1
625215	DRUGMATRIX: Calcium Channel Type L, Benzothiazepine radioligand binding (ligand: [3H] Diltiazem)	0	603	90	1
625217	DRUGMATRIX: Serotonin (5-Hydroxytryptamine) 5-HT2B radioligand binding (ligand: [3H] Lysergic acid diethylamide)	0	537	156	1
625218	DRUGMATRIX: Serotonin (5-Hydroxytryptamine) 5-HT2C radioligand binding (ligand: [3H] Mesulergine)	0	550	143	1
625219	DRUGMATRIX: Serotonin (5-Hydroxytryptamine) 5-HT3 radioligand binding (ligand: [3H] GR-65630)	0	660	33	1
625221	DRUGMATRIX: Serotonin (5-Hydroxytryptamine) 5-HT6 radioligand binding (ligand: [3H] Lysergic acid diethylamide)	0	598	95	1

Showing 1 to 10 of 362 entries Previous 1 2 3 4 5 ... 37 Next

Select database to download

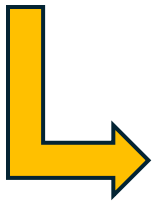
Select database:

BBB_curated

Download database

Select a database and click to download it as csv file.

Database



Resources

4. Resources
The details of the downloadable datasets available including references.

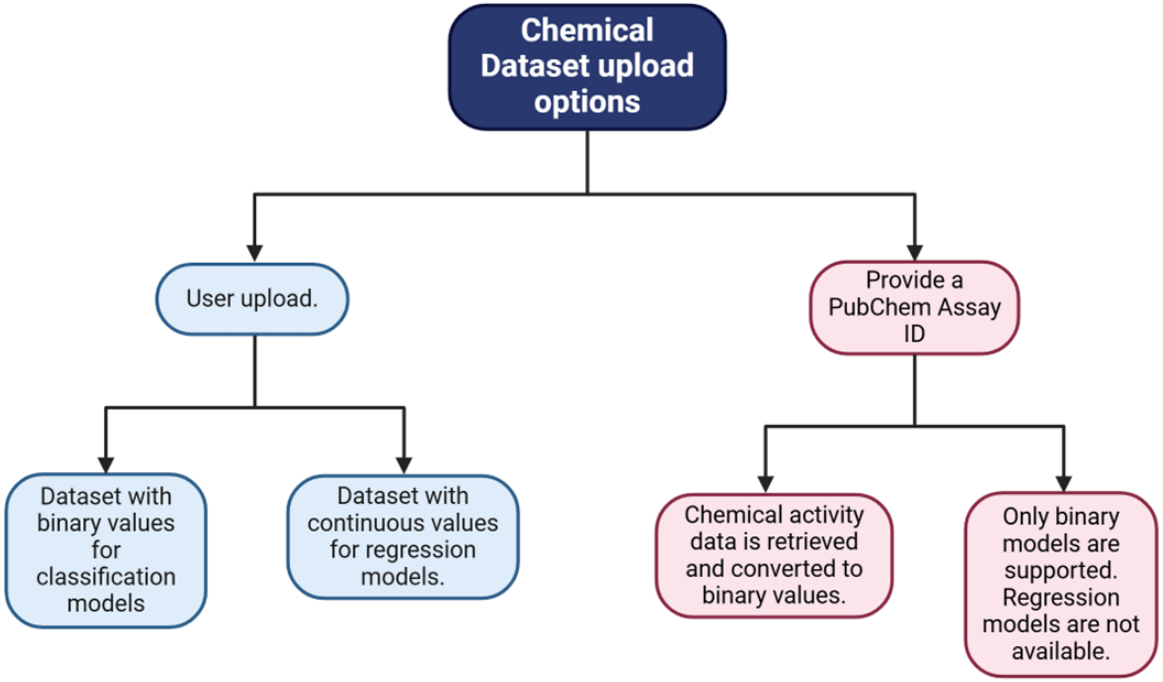
First few rows of the Resources Table

Curated Datasets

Dataset Name	Total # of Compounds	Data Type	Dataset Source	Dataset Description
BBB (Blood Brain Barrier)	438	logBB	Wang et al.	Compounds with experimental logBB values was compiled and curated using ChemAxon and CASE Ultra tools.
BCRP (Breast Cancer Resistance Protein)	395	μM (evidence of inhibition at 10 μM)	Sedykh et al. Zhao et al.	The BCRP dataset was curated for experimental consistency and structural quality, and filtered to include only reliable binary classification labels for substrates and inhibitors.
Bioavailability	1159	oral bioavailability (%F)	Kim et al.	Compiled across public and literature sources. Chemical structures were standardized, and %F values were harmonized to resolve discrepancies.
BSEP (Bile Salt Export Pump)	725	μM (evidence of inhibition at 100 μM)	Zhao et al.	Collected from publicly available experimental data. Structures were curated and standardized to ensure consistency and dataset includes binary labels.
Cancer (Human Oral Carcinogenicity)	342	Binary, 0=Non-Carcinogen; 1=Carcinogen	Chung et al.	342 unique organic compounds from the EPA's IRIS database, labeled as carcinogenic or noncarcinogenic based on oral slope factor (OSF), a quantitative measure for oral cancer risk.
Cosmetics	4129	---	Chung et al.	Cosmetic dataset collected from COSMOS Cosmetics Inventory knowledge base.
DART (Developmental and Reproductive Toxicity)	1452	Oral Developmental, Inhalation Maternal, ToxRefDB Maternal	Ciallella et al.	Collected from U.S. EPA's in vivo prenatal developmental toxicity studies in rats and rabbits based on oral or inhalation studies.
Drugbank	8055	---	Chung et al.	Collected from DrugBank database.

Cheminformatics

Upload or Retrieve datasets



5. Upload or Retrieve datasets

Data can be in the Comma-Separated Values (CSV) or Structure Data Format (SDF) format to upload. Sample files provided. You can upload or retrieve up to 1000 chemicals. Instead of uploading a dataset, you may also import structure-activity information from PubChem by entering the PubChem Assay Identifier (AID).

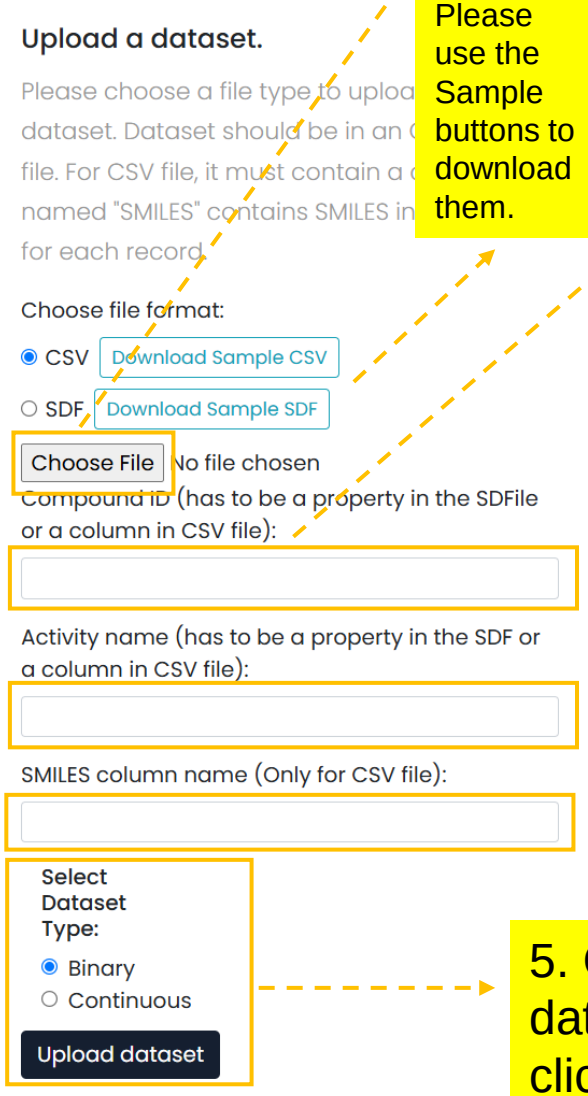
1. Upload a dataset (eg: sample_dataset.csv).

2. eg: cid.

Please use the Sample buttons to download them.

3. eg: Activity_Binary.

4. eg: SMILES.



5. Choose dataset type and click on Upload dataset.

*Accepts up to 1000 chemicals.

A sample file for Upload Dataset looks like this.

A	B	C	D
cid	SMILES	Activity_Binary	Activity_Reg
11	C(CCl)Cl	1	0.86
13	C1=CC(=C(C=C1Cl)Cl)Cl	0	0.31
174	C(CO)O	0	0.5
180	CC(=O)C	0	-0.02
240	C1=CC=C(C=C1)C=O	0	-1.11
241	C1=CC=CC=C1	1	-1.11
243	C1=CC=C(C=C1)C(=O)O	0	0.69
263	CCCCO	0	-0.22
299	C1(=O)C2(C3(C4(C1(C5(C2(C3(C(C45Cl)(Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	0	0.32
335	CC1=CC=CC=C1O	0	1.4
342	CC1=CC(=CC=C1)O	0	-0.16
712	C=O	0	0.02
727	C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl	1	0.38
887	CO	0	0.03
931	C1=CC=C2C=CC=CC2=C1	0	-0.15
949	CN(C)C1=CC=CC=C1	0	0.36
992	C1(=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl)O	1	-0.14
996	C1=CC=C(C=C1)O	0	0.95
1049	C1=CC=NC=C1	0	0.48
1140	CC1=CC=CC=C1	0	-0.05
1480	C1=C(C(=CC(=C1Cl)Cl)Cl)OCC(=O)O	0	-0.05
1486	C1=CC(=C(C=C1Cl)Cl)OCC(=O)O	0	-0.12
1489	C1=CC(=C(C=C1Cl)Cl)OCCCC(=O)O	0	-0.15
1493	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	0	-0.37
1982	CC(=O)NP(=O)(OC)SC	0	-0.84

Import a PubChem Bioassay.

Instead of uploading a dataset, you may also import structure-activity information from PubChem by entering the PubChem Assay Identifier (AID) below.

Enter PubChem AID (eg: 1259248):

Import dataset

Please check in Task option if the job is complete.

1. Enter an AID and click to retrieve the dataset

*Retrieves up to 1000 random chemicals. 500 actives and 500 inactives.

Selected dataset display once uploaded.

Upload a dataset.

Please choose a file type to upload a new dataset. Dataset should be in an CSV or SDF file. For CSV file, it must contain a column named "SMILES" contains SMILES information for each record.

Choose file format:

- (•) CSV — Download Sample CSV
- ( ) SDF — Download Sample SDF

Choose File — No file chosen

Compound ID (has to be a property in the SDFile or a column in CSV file):

Activity name (has to be a property in the SDF or a column in CSV file):

SMILES column name (Only for CSV file):

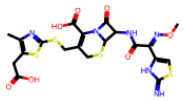
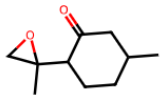
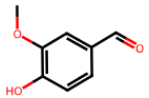
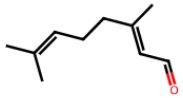
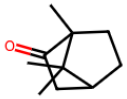
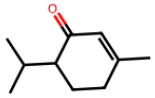
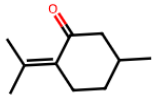
Select Dataset Type:

- (•) Binary
- ( ) Continuous

Upload dataset

Select dataset: sample_dataset_Binary

Show 10 entries — Search:

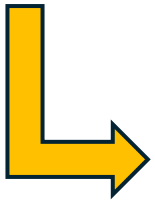
Chemical	Activity	Structure
TOX-1823	1	
TOX-1678	1	
TOX-1695	1	
TOX-1694	1	
TOX-1693	1	
TOX-1692	1	
TOX-1691	1	

Showing 1 to 10 of 1,000 entries — Previous 1 2 3 4 5 ... 100 Next

Download or remove the selected dataset

Remove dataset — Download dataset as CSV file

Cheminformatics



Curator

6. Curator

Cleans the chemical structures and prepares them for next steps such as model generation by the following steps:

i. Check and clean chemical structures.
ii. Standardize chemical structure representation (e.g, updating valencies, removing charges, etc.).
iii. Strip salts and remove mixtures by keeping the largest organic component.
iv. Merge or remove duplicated structures.

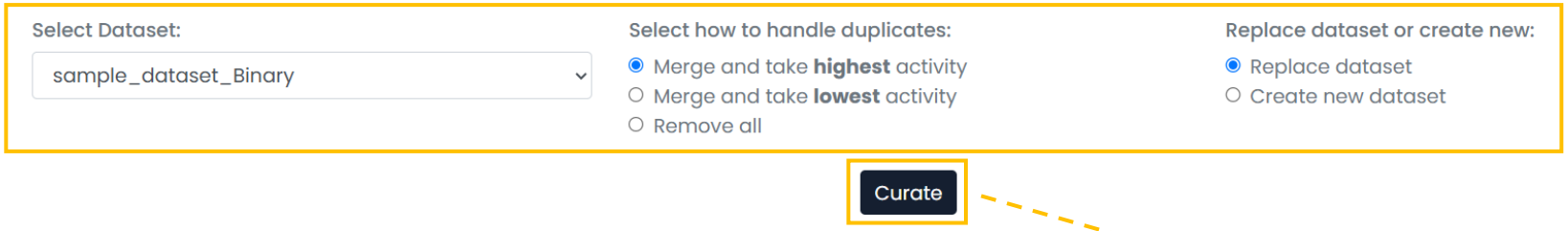
Please check in task if the job is complete.

Chemical curator

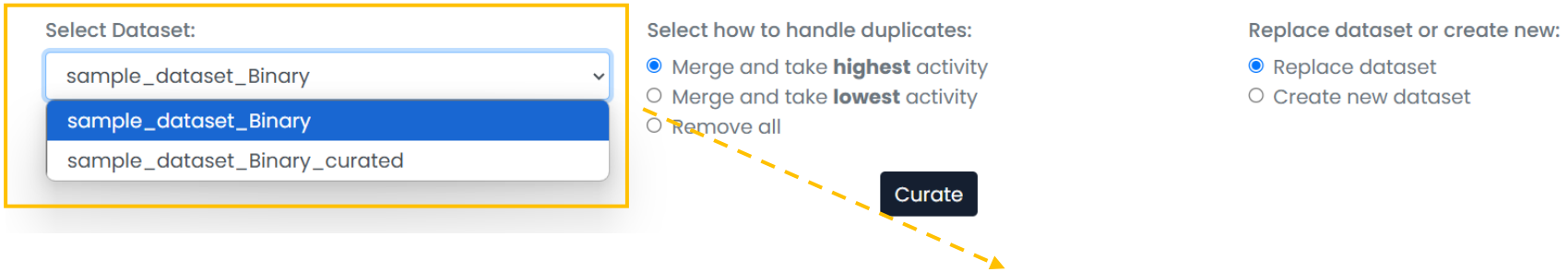
Proper chemical curation is a crucial step in Quantitative Structure-Activity Relationship development. This module cleans chemical structures and prepares them by using the following steps:

1. Check and clean chemical structures.
2. Standardize chemical structure representation (e.g, updating valencies, removing charges, etc.).
3. Strip salts and remove mixtures by keeping the largest organic component.
4. Merge or remove duplicated structures.

1. Select your dataset.

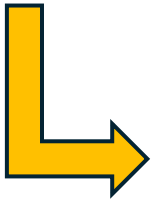


2. Click to run the curation.



A file named sample_dataset_Binary_curated is generated if ‘create new dataset’ option was chosen.

Cheminformatics



Principal Component Analysis

7. Principal Component Analysis

Principal Component Analysis (PCA) is a dimension reduction technique helps visualizing chemical space.

Principal Component Analysis

Principal Component Analysis (PCA) is a dimension reduction technique useful for visualizing chemical space. Select a dataset and click "Perform PCA" to visualize its chemical space. Chemicals will be colored according to their assigned activity (active, 1: red; inactive, 0: blue).

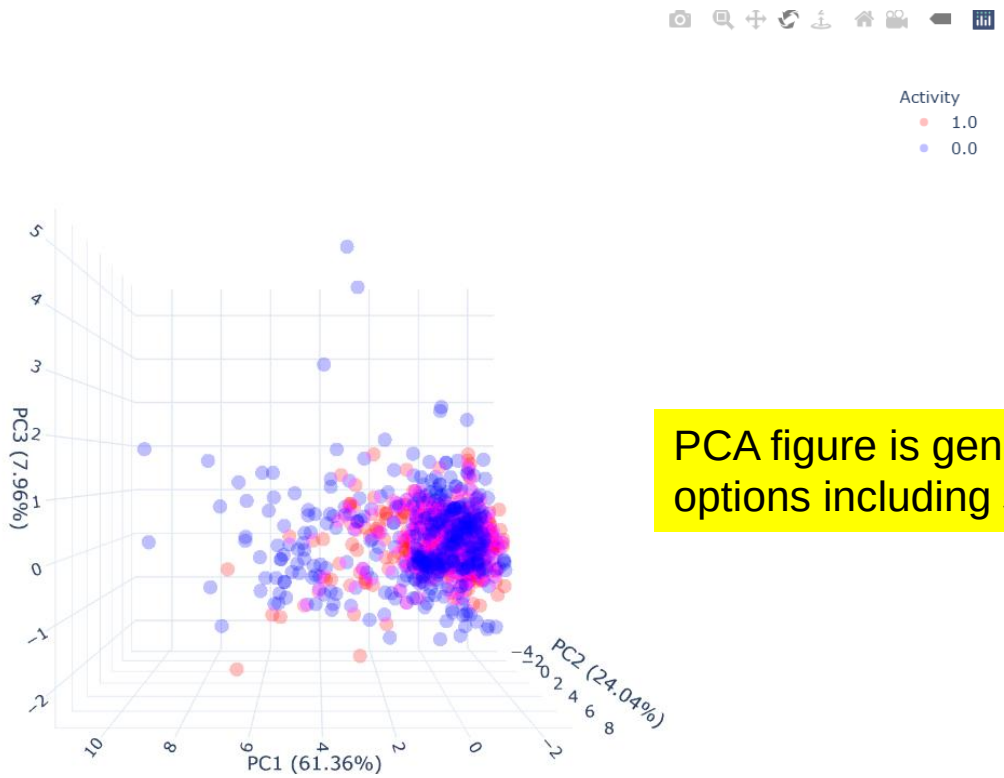
Select dataset:

sample_dataset_Binary

1. Select your dataset.

Perform PCA

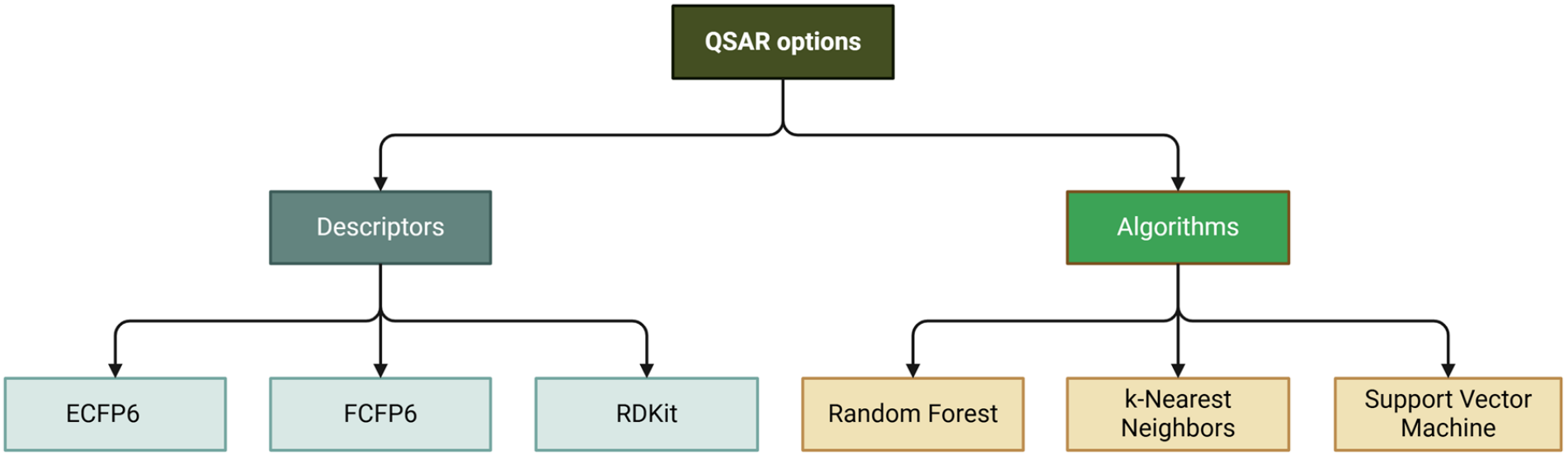
2. Click to generate PCA plot.



PCA figure is generated like shown with many options including save and zoom.

Cheminformatics

QSAR Builder

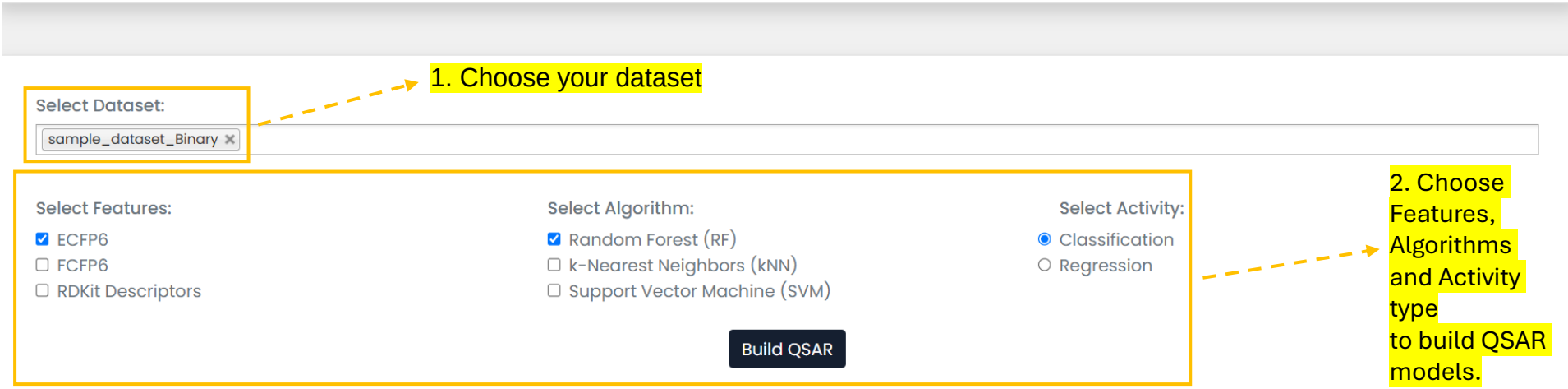


8. QSAR Builder

Create QSAR models using a variety of descriptors and algorithms with either a user-uploaded dataset or a dataset obtained by providing a PubChem Assay ID.

QSAR Builder

Quantitative Structure-Activity Relationship (QSAR) models are statistical models relating chemical structures to observed biological activitiies. A model is defined in this tab as a pair of features (e.g., ECFP6 fingerprints) and a machine learning algoritm (e.g., Random Forest). A QSAR model can be built by selecting a dataset, feature set, and machine learning algorithm and pressing the "Build QSAR" button. Depending on numerous factors, modeling training can take a while.



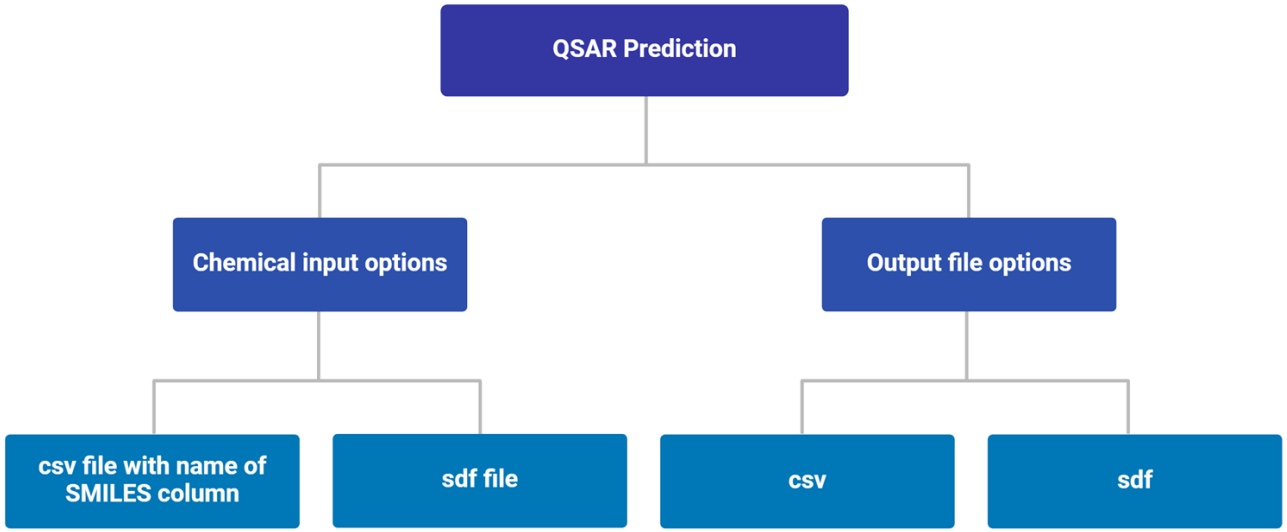
Trained Models

3. Check the evaluation metrics of your model.

Model	Type	Classification-Accuracy	Classification-F1 Score	Classification-Precision	Classification-Recall	Classification-Specificity	Regression-R2 Score	Regression-Max Error	Regression-Mean Squared Error
sample_dataset_Binary-ECFP6-RF-Classification	Classification	0.72	0.75	0.71	0.81	0.63	None	None	None

Cheminformatics

QSAR Predict



9. QSAR Predict

Predict toxicity for new chemicals using user-developed models.

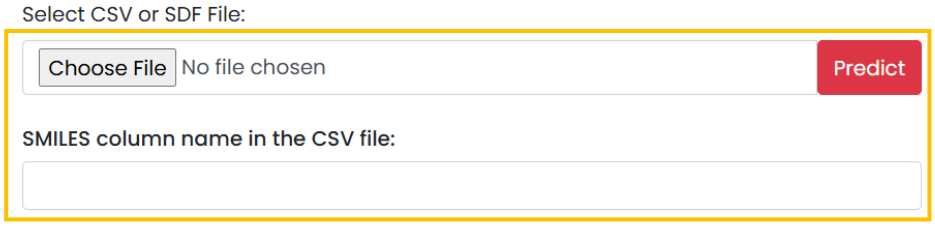
QSAR Predict

In this tab, you can select a previously built QSAR model(s) to make predictions on a set chemicals. After prediction, the modified CSV or SDF file will be directly downloaded to the user's computer.

*Accepts up to 100 chemicals.

1. Select QSAR your QSAR model.

2. Select an output format.



3. Choose a file eg: Prediction_dataset.csv and enter eg: SMILES, then click on Predict.

An output file eg: Prediction_dataset_predicted.csv is downloaded with a new column eg:sample_dataset_Binary-ECFP6-RF-Classification_Prediction contains predicted scores for the chemicals.

10. Contact us

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Questions, comments, and general inquiries can be emailed to toxiverse.help@gmail.com.

11. About us

The Zhu Lab uses cheminformatics algorithms, workflows, and other computational tools to model chemical toxicity, ADME (Absorption, Distribution, Metabolism, and Excretion), and other biological activities. These models support regulatory chemical toxicity assessments and the computer-aided drug discovery (CADD) process.

ZHU LAB

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