**Toxicity Prediction Challenge using Machine learning models**

Steps to install anaconda and packages:

* Download Anaconda
* Install Anaconda in your system
* Open Anaconda Navigator
* Open Jupyter Notebook from the Anaconda Navigator
* Open Conda Terminal and run below commands one by one

1. pip install rdkit-pypi
2. pip install catboost
3. pip install sklearn

Steps to run the file:

* Dataset and Code are available in below link

Google Drive:

<https://drive.google.com/drive/folders/1YfKDTzhs4Ocsf03LjEKoO35kFNK-s1im?usp=sharing>

Git Hub:

<https://github.com/karthikreddymarapa/Toxicity-Prediction-Challenge.git>

* I already shared two datasets with 209 features exported into in it . To run Descriptors.ipynb file it will take around 2 hours to run.
* If you want run this file , open the Descriptors.ipynb file first and click on cell and select Run all option.
* Then run the ModelCat file by placing the train\_I and test\_I csv files in the same path where we are running the python file.
* I Commented out the Grid Search CV code in this file , because it will take around one hr to execute.if you want to run it please un comment it.
* Then click on cell and select Run all option.

Graphical user interface, text, application

Description automatically generated

Notes: Please keep the dataset and the jupyter file in the same location