**THE TOXICITY PREDICTION CHALLENGE II**

**(CSCI 555-DATA MINING AND MACHINE LEARNING)**

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
2. pip install catboost
3. pip install sklearn

Version of Anaconda Jupyter Server Information:  
  
The version of the notebook server is: **6.4.5**  
The server is running on this version of Python: 3.9.7

Steps to run the file:

* Dataset and Code are available in below link:
* Open the **Toxicity\_Code1.ipynb** file first and click on cell and select Run all option.

**Code Links:**

**Kaggle Container Best Submission Link:**

[**https://www.kaggle.com/code/vinodkumar2021/x2021gml-best-score**](https://www.kaggle.com/code/vinodkumar2021/x2021gml-best-score)

**Git Hub:**

[**https://github.com/VinodKumar86/Toxicity\_Prediction\_202106148**](https://github.com/VinodKumar86/Toxicity_Prediction_202106148)

**Google Drive Link:** [**https://drive.google.com/drive/folders/1tEJ024WJaT98PlpV6l60siCpieWxN0U1?usp=share\_link**](https://drive.google.com/drive/folders/1tEJ024WJaT98PlpV6l60siCpieWxN0U1?usp=share_link)

Graphical user interface, application

Description automatically generated

**Note:** Please keep the dataset and the jupyter file in the same location.