**PyRegX: A Multivariate Regression Plug-in for PyMol**

***PyRegX*** is a GUI-based plugin designed to perform robust ***Multiple Linear Regression (MLR)*** analysis on structured datasets directly from PyMol. Built with Customtkinter, it allows users to load datasets, define regression targets, validate models using statistical metrics, and export results-all without writing code.

**🔍 Key Features**

* 📂 Load training and test datasets in ***.CSV*** format
* 🧹 Automatic removal of null-valued columns
* ✍️ Select dependent (***Y***) variable *via* dialog
* 📈 Run multivariate regression using ***statsmodels.OLS***
* ✅ **Validate models with**:
  + ***Internal Metrics:*** *R², Adjusted R², MAE, RMSE, VIF, PRESS, SEE*
  + ***External Metrics:*** *Q² (f1, f2), MAE, RMSE*
  + ***Cross-Validation:*** Leave-One-Out *Q²* and *MAE*
* 📝 **Export**:
  + Statistical summaries (txt)
  + Prediction tables (\_train.csv, \_test.csv)
* 📊 **Visualization**:
  + Correlation Heatmap
  + Observed vs Predicted Scatter Plot
* 🧩 **Easy integration as a PyMol Plug-in** (Menu -> Plugin -> PyRegX gui)

***NOTE: The Index column must be at the first column of the input files.***

**📦 Dependencies**

Ensure the following packages are installed in your Python environment:

* os, sys, subprocess, warnings
* NumPy, Pandas
* Scikit-Learn, statsmodels
* Seaborn, Matplotlib
* Tkinter
* Customtkinter (for modern GUI components)
* PyMol (for integration)

**⚙️ Installation**

**Option 1: Install in PyMol environment (manual)**

1. Place the plugin .py file in your PyMol plugins folder (e.g. ~/.pymol/startup/ or via Plugin Manager).
2. Launch PyMol and navigate to **Plugin > Manage > Install** and select the .py file.
3. PyRegX will appear in the **Plugin** menu.

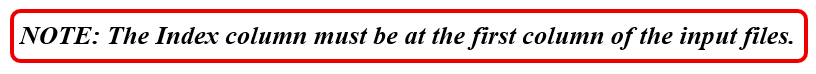
**Option 2: Install required Python dependencies**

If you're not using a pre-configured Python environment, install dependencies with pip:

$ pip install pandas numpy scikit-learn statsmodels matplotlib seaborn customtkinter

**🚀 Usage Workflow**

1. **Launch PyRegX GUI** from PyMol:  
   *Plugin → PyRegX gui (v0.23)*
2. **Load Training Dataset**
   * Click *"Load Training Data"* and select a ***.csv*** file
   * The file must contain both independent and dependent variables
3. **Load Test Dataset**
   * Click *"Load Test Data"* and select a .csv file with the same structure
4. **Enter Dependent Variable (*Y*)**
   * Click *"Enter Dependent Column"*
   * Provide the exact column name to be predicted
5. **Select Output File**
   * Click *"Select Output File"* to specify where to save results
6. **Run Analysis**
   * Click *"Run Analysis"*
   * Generates regression summary, validation metrics, and prediction output
7. **Visual Output**
   * Correlation heatmap and scatter plot will pop up post-analysis



**📊 Statistical Metrics Used**

**✅ Internal Validation**

* ***R² (Coefficient of Determination/Squared correlation coefficient)***  
  Measures how well the regression model explains the variance.



* ***Adjusted R²***Accounts for number of predictors:

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* ***SEE (Standard Error of Estimate)***

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* ***Q2LOO (Internal Leave-One-Out cross-validated coefficient of determination)***Parameter indicates model fit under cross-validation (*See later*).
* ***PRESS (Predicted Residual Error Sum of Squares)***Parameter indicates model fit under cross-validation.
* ***MAE (Mean Absolute Error)****,* ***RMSE (Root Mean Square Error)***  
  Parameter to quantify average prediction error.
* ***VIF (Variance Inflation Factor)***Parameter for multicollinearity assessment

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**📤 External Validation**

* ***Q² (f1)*** **/** ***R2Pred***

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* ***Q² (f2)* / *R2Test***

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**🔁 Cross Validation**

* ***Leave-One-Out Q² (Internal Leave-One-Out cross-validated coefficient of determination)***  
  Validates the model with each observation removed once. ***Q2LOO*** = ***R2*** (on predicted *vs* actual in *LOO* setting)

**📚 References**

* ***Statistical References***
* Banerjee, Adhikari, Amin and Jha (2020). *Structural exploration of tetrahydroisoquinoline derivatives as HDAC8 inhibitors through multi-QSAR modeling study*, Journal of Biomolecular Structure and Dynamics, 38(5):1551-1564. **DOI:** 10.1080/07391102.2019.1617782.
* Draper, N.R. & Smith, H. (1998). *Applied Regression Analysis* (3rd ed.). **DOI:**10.1002/9781118625590.
* Montgomery, D.C., Peck, E.A., & Vining, G.G. (2012). *Introduction to Linear Regression Analysis.* **DOI:**10.1111/insr.12020\_10
* Golbraikh, A. and Tropsha, A. (2002) *Beware of q2!* Journal of Molecular Graphics and Modelling, 20, 269. **DOI:** 10.1016/s1093-3263(01)00123-1.
* Roy, Kar, and Das (2015). *Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment*. **DOI:** 10.1016/C2014-0-00286-9.
* ***Software, Tools and Modules***
* <https://pymol.org/>
* <https://github.com/schrodinger/pymol-open-source>
* <https://numpy.org/>
* <https://pandas.pydata.org/>
* <https://scikit-learn.org/>
* <https://www.statsmodels.org/>
* <https://github.com/TomSchimansky/CustomTkinter>
* <https://docs.python.org/3/library/tkinter.html>
* <https://matplotlib.org/>
* <https://seaborn.pydata.org/>

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**Version:** 0.23

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