ECMC-P 2025 Conference

The 1st International Electronic Conference on Medicinal Chemistry and Pharmaceutics

01–30 November 2025 | Online

MDPI

CODRUG: An open-source graphical interface for Ligand-Based Drug Discovery using QSAR and Machine Learning

Moisés Maia Neto[1]*; Bernardo Mussa[1]; Raul Edison Luna Lazo[1]; Roberto Pontarolo[1,2]*

[1] Postgraduate Program in Pharmaceutical Sciences, Federal University of Paraná, Curitiba 80210-170, Brazil.

[2] Department of Pharmacy, Graduate Program in Pharmaceutical Sciences, Federal University of Paraná. Curitiba 80210-170, Brazil.

*E-mail: moisesmaia@ufpr.br, pontarolo@ufpr.br

INTRODUCTION & AIM

Ligand-based drug design (LBDD) approaches, particularly quantitative structure–activity relationship (QSAR) models, are well-established tools in modern drug discovery[1,2]. Their relevance has grown with advances in machine learning (ML) and neural networks, coupled with the expansion of structural and bioactivity databases[3]. However, applying these big data methods remains challenging for researchers in small laboratories due to the need for programming skills, integrated development environments (IDEs), or costly proprietary software. The development of open-source, user-friendly, and flexible graphical interface CODRUG, aims to overcome these barriers and democratize access to computational drug design tools.

METHOD

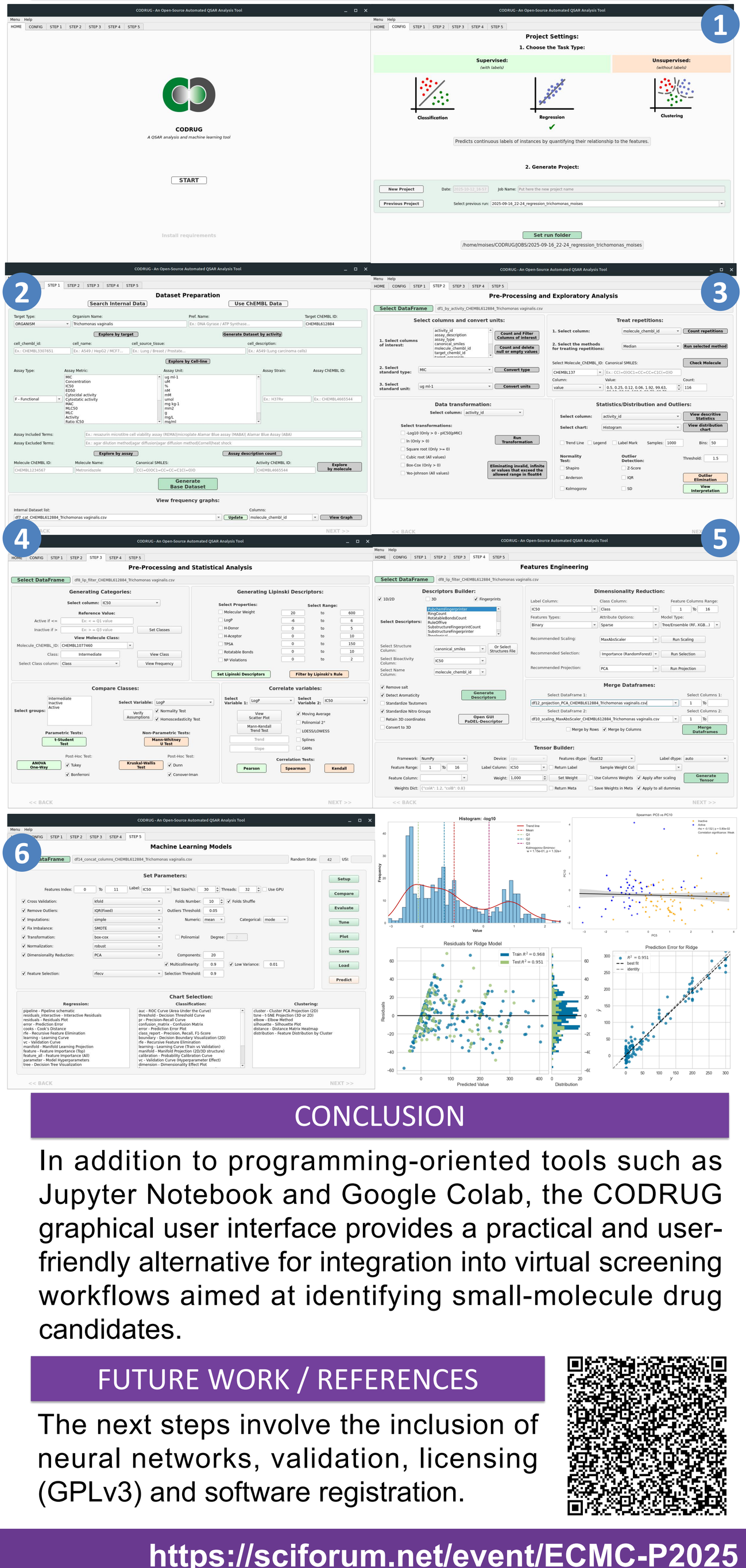
Development:

OS	IDE	Language	Framework
Linux Mint *21.3*	VS Code *1.105.0*	Python *3.10.12*	PyQt5 *5.15.11*

Workflow and Main Packages[4,5,6]:

1. **Project Settings:** Jobs; Regression; Classification; Clustering
2. **Dataset Preparation:** ChEMBL; pandas
3. **Preprocessing:**
4. **Exploratory and Statistical Analysis:** NumPy; matplotlib; RDKit
5. **Features Engineering:** PaDEL - Descriptor; TensorFlow; PyTorch
6. **ML Models:** *Train, Test, Validation and Predictions.* PyCaret; scikit learn

RESULTS & DISCUSSION



CONCLUSION

In addition to programming-oriented tools such as Jupyter Notebook and Google Colab, the CODRUG graphical user interface provides a practical and user-friendly alternative for integration into virtual screening workflows aimed at identifying small-molecule drug candidates.

FUTURE WORK / REFERENCES

The next steps involve the inclusion of neural networks, validation, licensing (GPLv3) and software registration.