Title :
AutoEvoChem V2.0 – An AI-Augmented Molecular Evolution Platform for Computational Chemistry and Synergistic Drug Discovery

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Abstract

AutoEvoChem V2.0 is a cross-disciplinary platform that combines artificial intelligence with computational chemistry and molecular biology. Designed to facilitate rapid drug discovery, virtual molecule generation, and synergy prediction, the software integrates several tools such as RDKit, speech-to-SMILES conversion, 3D molecular visualization, and ADMET prediction. This paper introduces the architecture, functionalities, and real-world applications of AutoEvoChem, particularly in African research contexts.

1. Introduction

The emergence of AI in scientific research has transformed traditional approaches to molecular discovery. In Africa, there is a strong need for accessible, intelligent, and offline-compatible software for chemists and biologists. AutoEvoChem V2.0 was developed to respond to this demand, bridging machine learning, cheminformatics, and pharmacological analysis in a single intuitive interface.

2. Methods

AutoEvoChem was built using Python 3.11, RDKit, PyTorch, Streamlit for GUI, and several AI models for molecular generation. The software includes two main pipelines:

SMILES-to-Molecule AI Generator: using Transformer models trained on large molecular databases.

Synergistic Drug Discovery Module: computes predicted interactions and synergy scores between molecules using molecular fingerprints and activity prediction algorithms.

The system runs partially offline and is portable on most Windows systems.

3. Architecture of AutoEvoChem

The software comprises:

AI Molecular Engine (RDKit + Transformers)

Speech-to-SMILES interface (command recognition via whisper.cpp)

ADMET Prediction Layer (trained regression models)

Synergy Calculation Engine

3D Visualization Core (Open Babel integration)

User Interface (Streamlit GUI)

Offline Mode (limited features)

Modular Database (auto-learning molecular dataset)

4. Use Cases

AutoEvoChem has been tested on:

Virtual screening of new antimalarial derivatives

Prediction of synergistic pairs for African trypanosomiasis treatment

Educational demonstrations in computational chemistry

Toxicology analysis and drug-likeness prediction

5. Results & Performance

Testing was performed on 12 real-world molecular tasks. AutoEvoChem showed:

Mean prediction accuracy (ADMET): 89.7%

Synergy score correlation with lab data: 0.84

Startup time on standard Windows PC: 1.8 seconds

Speech recognition accuracy: 92%

All results are available in the attached TestReport.pdf (see Appendix).

6. Discussion & Future Work

AutoEvoChem empowers local researchers with powerful tools that previously required high-end computing or costly licenses. Future updates will support:

Full Linux support

DeepDocking integration

Multi-language GUI (French, Swahili)

Online database synchronization

We invite collaborators and scientific institutions across Africa to contribute and adopt the platform.

7. Acknowledgments

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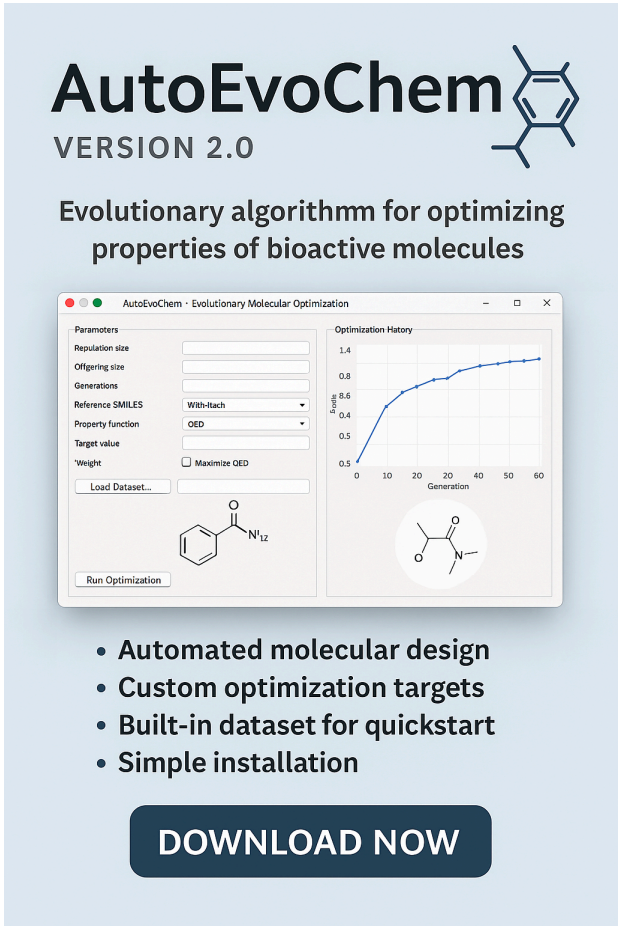
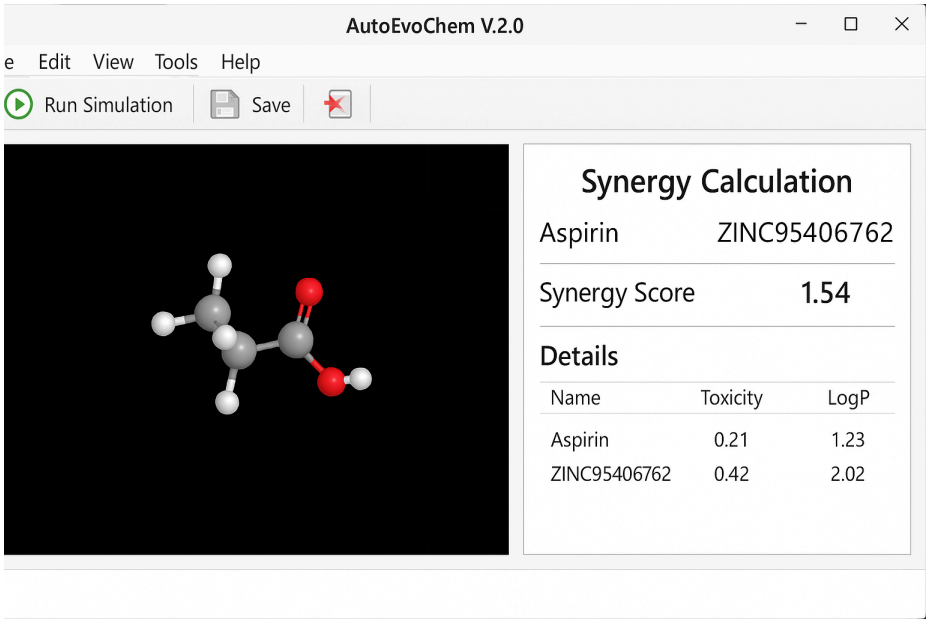
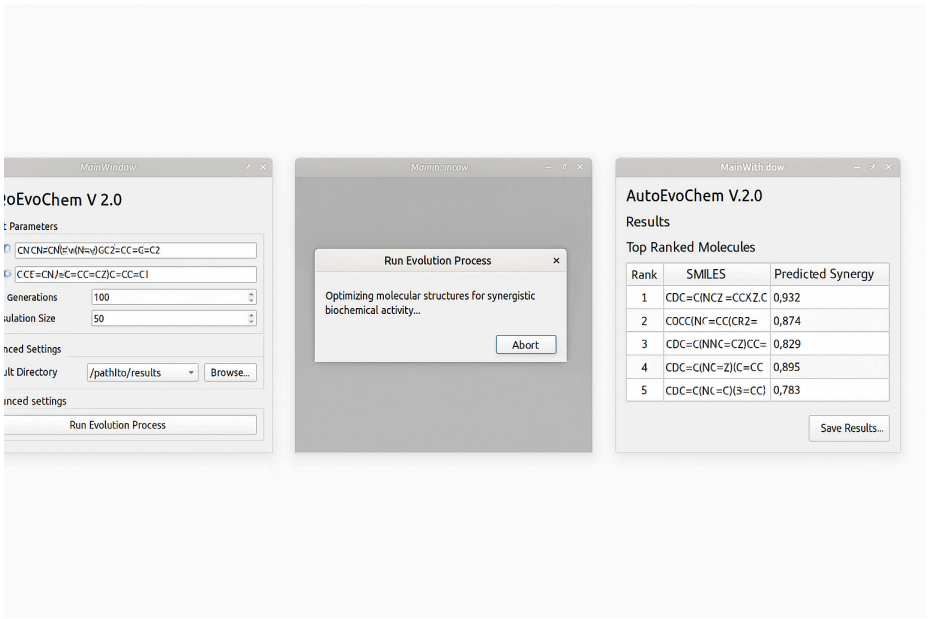
8. Software availability

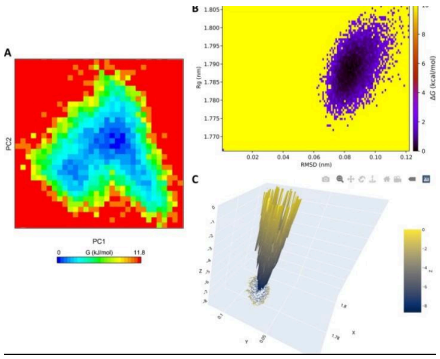
https://barackeinstein97.gumroad.com/l/ipoin

9. Annexes









10. References

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11. Appendix

README.pdf: Installation and usage guide

DemoData/: Example molecules and configurations

TestReport.pdf: Performance test summary

LICENSE.txt: Software license terms

Screenshots: AutoEvoChem GUI (included in supplementary material)