

Decoding Protein Dynamics using Artificial Intelligence

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1 Objective: to leverage the protein engineering with the data extracted from molecular dynamics simulations via state-of-the-art Artificial Intelligence (AI) methods.

Proteins form the basis of life, with all its great variety and efficiency. **Wide range of functions** in living organisms, from catalyzing metabolic reactions to building structures in cells and tissues.

Protein engineering develops advanced and valuable proteins for a vast range of applications in various fields.

Proteins are moving!!! **WOW!**

2 Understanding Dynamics → Understanding Functionality

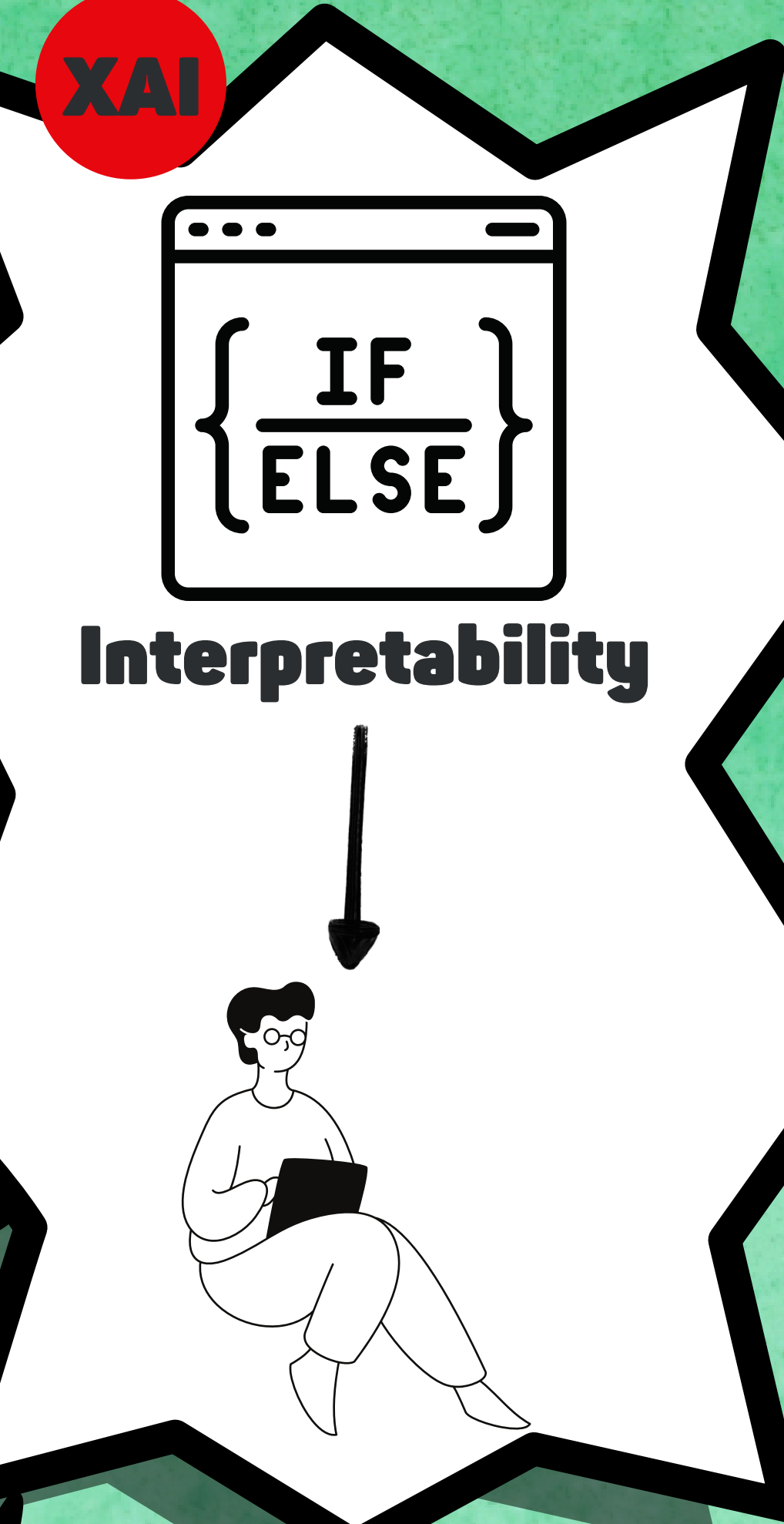
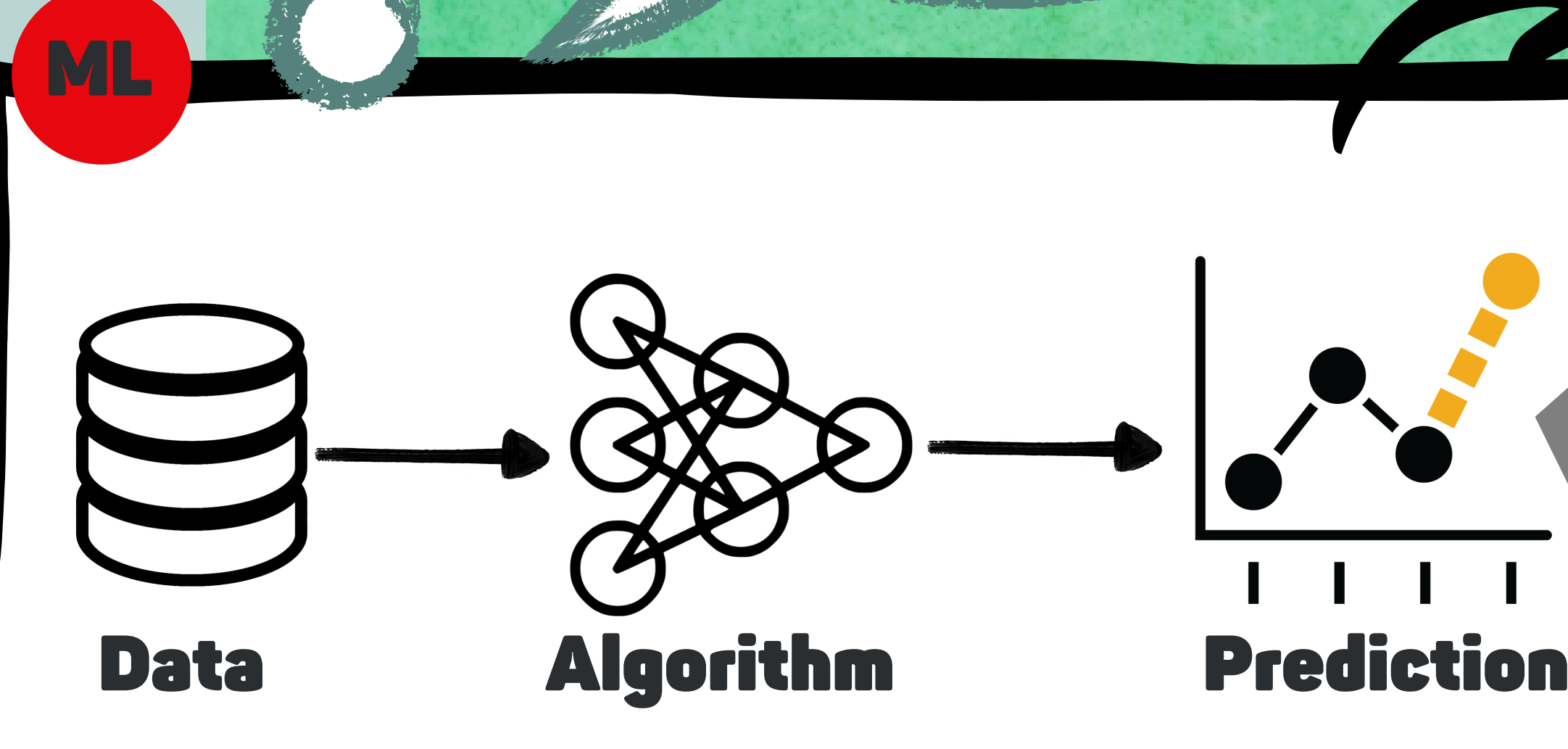
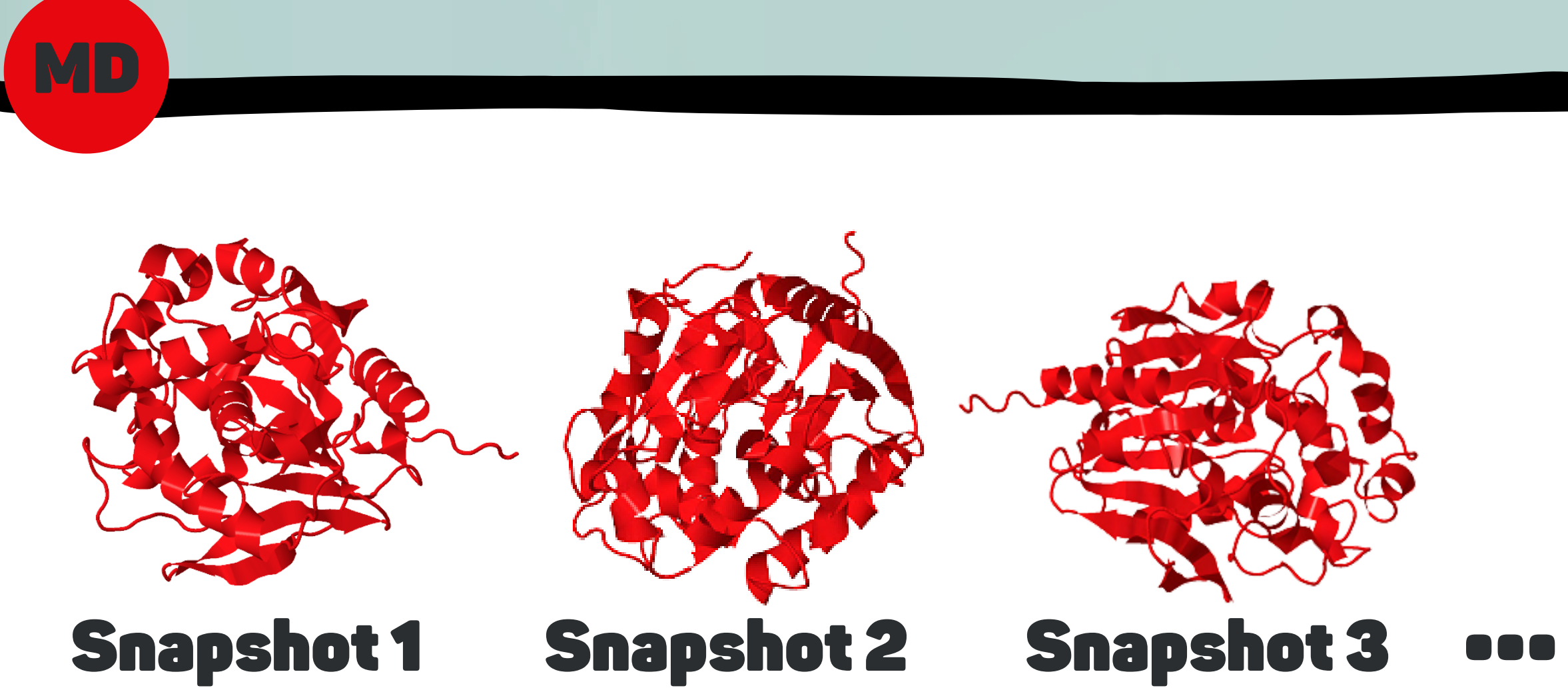
Molecular Dynamics (MD) a method for analyzing the physical motion of atoms and molecules.

Results of MD are sequential snapshots of states of the biomolecule at specific time intervals, represented by atomic 3D coordinates.

Tremendous amount of data
Visual inspection insufficient
Manually selected metrics
Human bias

what is the solution?

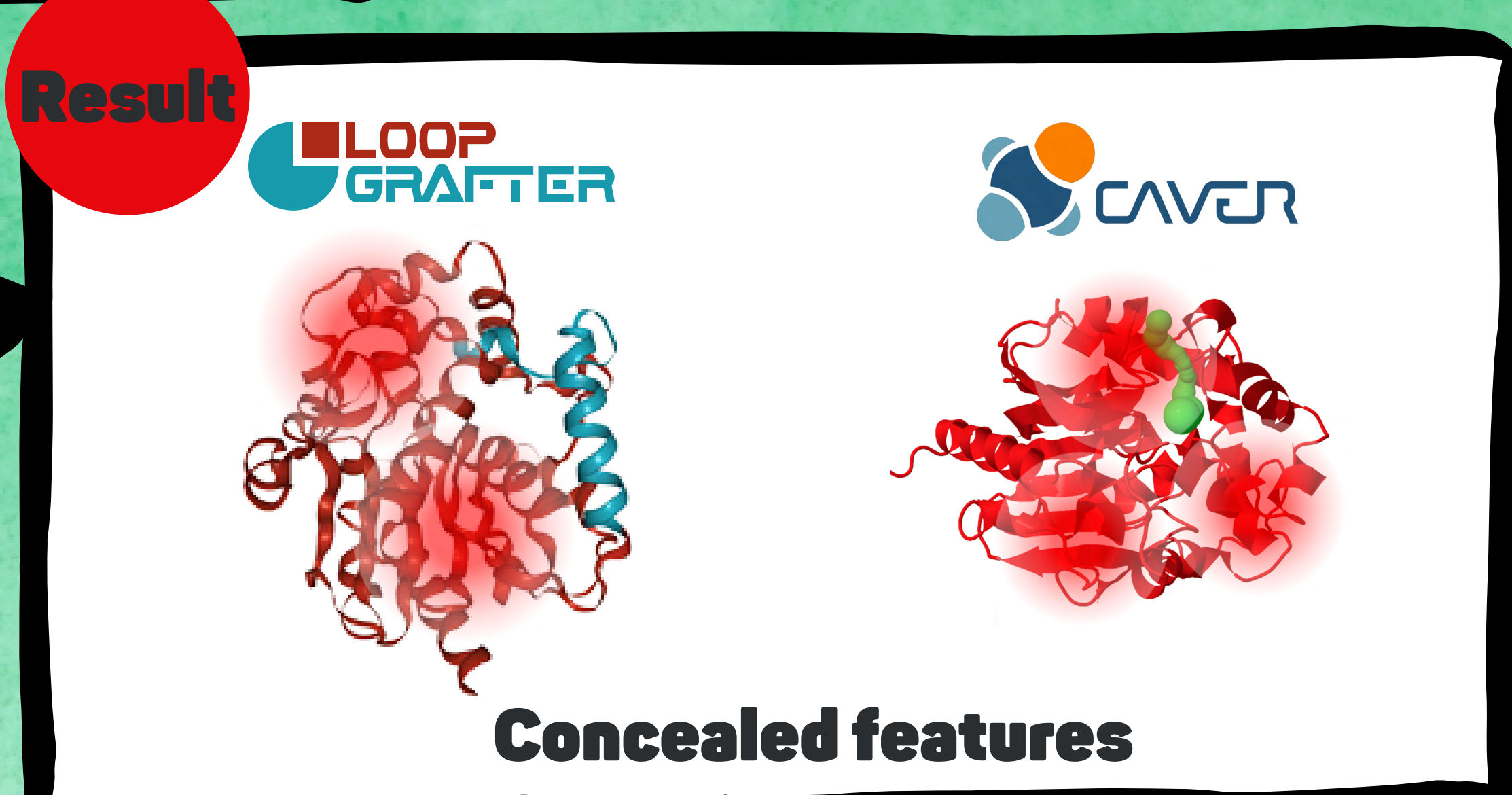
MACHINE LEARNING



3 Machine learning (ML) can help us!

But we need another solution to find **concealed features** in the proteins!

Yes! **Explainable Artificial Intelligence (XAI)**!

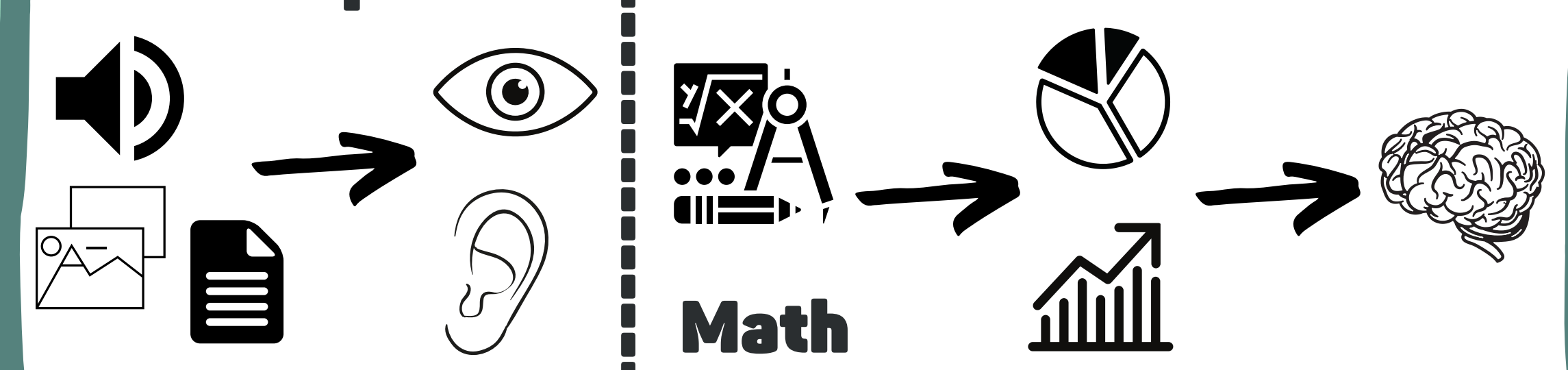


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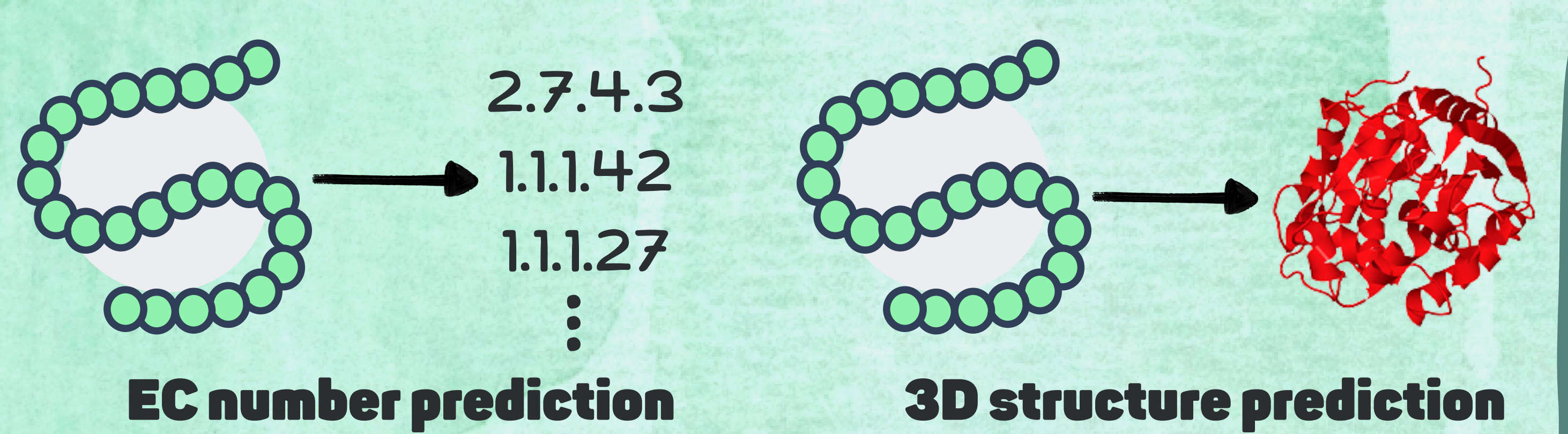
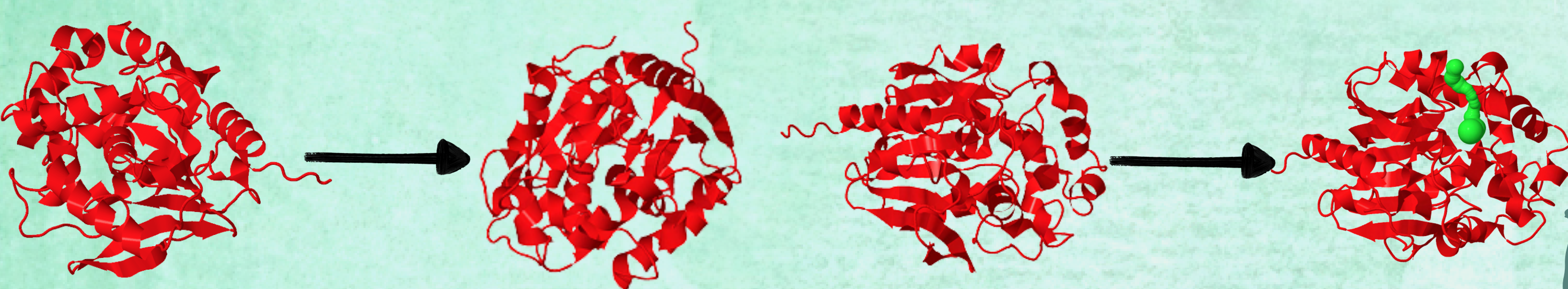
Two major XAI categories:

Perceptive

Mathematical



ML architecture transforms raw data into a training set to learn patterns and make decisions (predictions).
Different ML architecture: **CNN, RNN...**



5

CAVER rapid, accurate, and fully automated calculation of protein tunnels.

Current version does not benefit from available MD simulations.
Next steps: conduct MD simulations and their ML-based analyses

- tunnel motions
- various types of tunnels prediction
- best hotspots for protein engineering identification



LOOP GRAFTER transplants loops between two structurally similar proteins.

Current version uses a simple B-factor model based on the parameters calculated in X-ray crystal structures to analyze the dynamics of the loops.
Next steps: conduct MD simulations and their ML-based analyses

- identification of interlinked loops
- loop ranking according to the desired property

