

# ZYMVOL releases ZYMEVOLVER 2.0, a new generation of enzyme engineering software

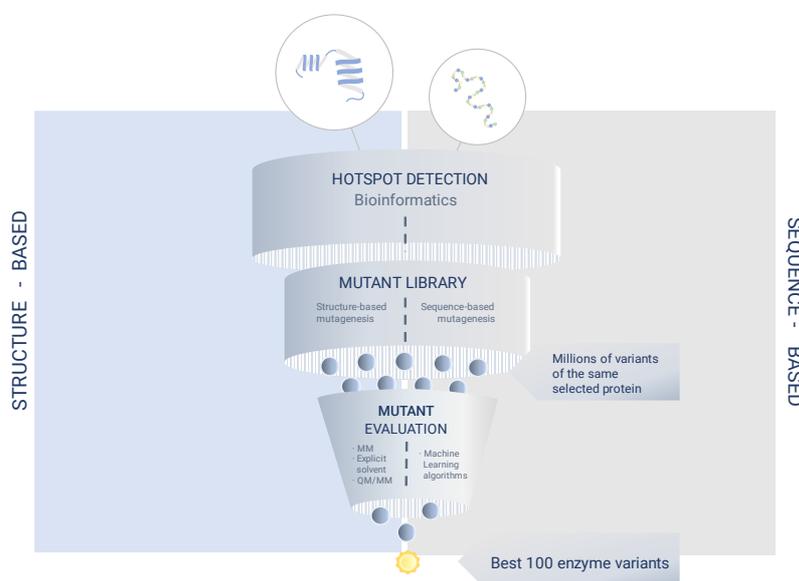
- *Machine Learning, Network Analysis and Modularity are some of the key features of the company's latest pipeline*

**Barcelona, November 29th 2021.** Under the framework of SME Phase2 project, UNLOCK-EDD, funded by EC Horizon 2020 Program, the biocatalyst discovery and development company ZYMVOL has released **ZYMEVOLVER 2.0., a new improvement of its *in silico* enzyme engineering software.**

With the advent of Artificial Intelligence, the ZYMVOL team has bet on upgrading its technology to stay at the vanguard of innovation in the protein engineering field.

The new release includes:

- **Machine learning algorithms:** When experimental data is provided by the customer, AI algorithms can be used to make more accurate predictions of mutations.
- **Network Analysis:** Through network analysis, enzyme hotspots can be identified. This allows to focus only on those residues with a potential effect on the activity, specificity, etc., reducing the number of residues to study (meaning faster simulations) and opening the door to include long-range mutations.
- **Quantum-mechanics removed from the main pipeline:** Faster simulations without losing predictability. It can still be included when it's critical.
- **Modularity:** Zymeolver2.0 has been refactored to make it a modular software. Now, it's easier and faster to include new technologies to the main program. For instance, Alphafold2 is being included to automatically build 3D structures, replacing/complementing homology modeling.



**ZYMVOL Senior Scientists Ryoji Takahashi and Ferran Sancho** are behind the development of this new version, which aims to tackle some of the most common challenges scientists face while conducting enzyme engineering projects.

“It represents a significant improvement in our technology. Since the simulations are performed quicker, scientists will have more time to broaden the sequence space exploration (including long-range mutations) and suggest more mutations per round (from 30->90)”, states **Ferran Sancho**. “This also increases the number of hits: with some customers, only long-range mutations have a positive impact on the enzyme activity. With ZYMEVOLVER 2.0, the number of successful projects also rises”.

For ZYMVOL, the release is seen as a natural step towards their continuous effort to advance its state of the art methods. “We are now able to have access to other, risky, not used till now enzymes, and we can face more challenging projects at lower risk”, states **Ryoji Takahashi**.

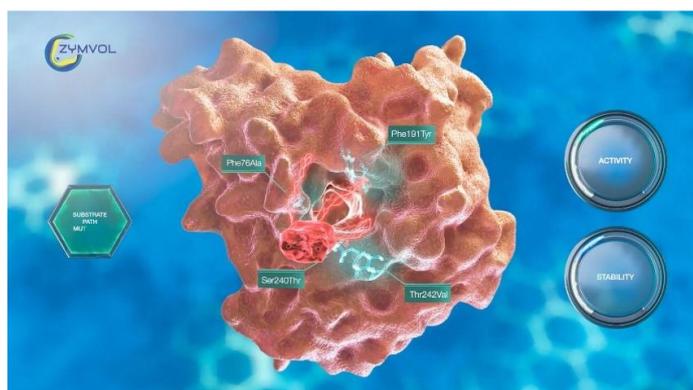
### Leading the way on Computational Enzyme Engineering

ZYMEVOLVER was the first software pipeline developed by ZYMVOL at the time of its foundation. It’s an *in silico* design (ISD) pipeline that combines multiple solutions from bioinformatics, protein design algorithms, and molecular modeling. It was created with the **goal of redesigning a desired enzyme** to efficiently catalyze the target reaction under the customer’s industrial conditions.

Enzyme properties such as activity, specificity and selectivity can be improved, but also enzyme stability (to temperature, pH, solvent, complex matrices, etc.).

The cornerstone of this technology is the combination of bioinformatics with reliable physics-based simulations that model the interactions between the substrate and the enzyme. Such simulations follow a funnel-like scheme with increasing complexity to gradually filter enzyme candidates.

Thanks to these features, ZYMEVOLVER is able to replace the often expensive and time-consuming enzyme evolution experiments with quick, thorough, accurate simulations. Since enzyme evolution takes place *in silico* (that is, in computers), **only a small selection (up to/average 300 candidates) requires being tested in the lab**. ZYMEVOLVER has been successfully used already in a wide number of projects with clients worldwide.



### EU-Powered Innovation

ZYMEVOLVER technology has been developed with the support of “**UNLOCK-EDD: UNLOCKing next generation computer guided Enzyme Discovery & Design**”, a project financed by SME Phase2 in the frame of Horizon 2020, the European Union’s research and innovation programme.

The Horizon 2020 program aims to ensure that Europe produces world-class science, removes barriers to innovation and makes it easier for the public and private sectors to work together in delivering innovation.

Through “UNLOCK-EDD”, ZYMVOL has taken on the challenge of becoming a reference in the computer-driven enzyme engineering market and converting molecular modelling into a commodity. Project goals are:

- To keep improving proprietary technology by implementing artificial intelligence approaches.
- The development of a computational pipeline for enzyme kits.
- The development of proprietary enzymes.

#### About ZYMVOL

[ZYMVOL Biomodeling SL](#) is a privately funded company specialized in *in silico* enzyme engineering. Founded in May 2017, the company currently has customers in more than 10 countries worldwide and is actively engaged in highly innovative and competitive R&D projects. In 2020, the European Commission awarded CEO Maria Fátima Lucas the [EU Prize for Women Innovators](#).

ZYMVOL’s mission is to expand the use of Green Chemistry in the industry by leading the way on computer-driven, enzyme engineering technology.

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