Workshop on Digital Bioeconomy: Convergence towards a bio-based society



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Computer Aided Enzyme Discovery and Engineering for Industrial Biocatalysis: From physics based MD to Machine Learning and AI

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Enzyme engineering by directed evolution allows the optimisation of virtually any enzyme into a powerful industrial catalyst, which can be conveniently applied under process conditions. However, due to time and cost limitations, enzyme discovery from (meta)-genomic diversity often fails to deliver high performance catalysts ready for industrial applications and enzyme variant screening under process conditions can only cover a very limited protein sequence space.

In order to overcome this limitation in Enzyme Discovery & Engineering, Enzymaster has developed the Bio-Engine®, a proprietary directed evolution platform with integrated computational enzyme identification/enzyme engineering toolbox BioNavigator®. This enables us to cover much larger sequence space using machine learning/AI for combining activity, 3D-structure and sequence information in our EM 2 L-platform for predictive in-sillico screening.

In this presentation I will show, how Enzymaster is utilizing it's digital toolbox in order to speed up our smart enzyme evolution platform BioEngine® by computer aided enzyme engineering. We combine high throughput screening and next generation sequencing for fast and reliable data generation with AI and machine learning approaches for virtual enzyme identification and screening.

Enzymasters aim is to deliver practical solutions enabled by a powerful combination of experimental and virtual screening to overcome the hurdle from idea to product in a future data driven bioeconomy.

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Consent

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