

Enzymes for Green and Clean Synthesis and Bioremediation

EMBLEM 2021-020

Challenge

- Increasing environmental awareness and regulation force industry to adapt their processes towards more environment friendly synthesis and effective wastewater treatment
- Enzymes carry out chemical processes with excellent chemo-, regio- and stereospecificity under the mild conditions of living cells without the requirement of high temperatures, pressure or toxic and are thus ideally suited to address these challenges
- With the tools for *in silico* enzyme discovery and development the most suitable enzyme candidates in a highly cost and time efficient manner are able to be identified

Commercial Opportunity

- EMBL offers opportunities in the fields of service provision, collaboration and co-development, and investment.

Technology

in silico enzyme discovery and development:

- The Discover Module identifies the most suitable enzymes from feasibility and value perspectives. Here, a high-throughput virtual screening of large chemical datasets against known enzyme chemistry is performed, data-mine known enzyme reactions, screen chemical market data and propose novel enzymatic transformations that is prioritised by similarity, value and ease of manufacturing.
- The Develop Module then identifies activity enhancing mutations with a Novel dynamic docking procedure. The desired substrate into the catalytic centre with alchemical methods is modeled and unfavourable clashes are resolved as the ligand is gradually switched on inside the enzyme binding pocket. The module is under continued development and testing for correlation between *in silico* predictions and *in vitro* observations on selected examples.

Contact

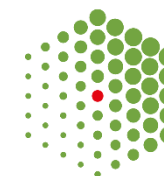
Dr. Birgit Kerber, kerber@embl-em.de

Key Inventors

Dr. Jonathan Tyzack
EMBL EBI

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Benefits:

The various search modes of the Discover Module allow:

- To identify valuable reactions for a known enzyme to maximize the substrate and product space of the existing enzyme portfolio
- To find the enzyme that represents the best starting point for the development of a novel biosynthesis or degradation/remediation reaction of interest
- To find a biosynthetic path to produce a chemical of interest starting from a simple commodity chemical (retrosynthetic search).
- To find a biosynthetic path to degrade a chemical of interest to a non-harmful substance (retrosynthetic search).

The Develop Module enables the fast and highly efficient optimization of enzyme activity towards a novel substrate while avoiding costly rounds of directed evolution. The activity enhancing mutations identified by the Develop Module can considerably increase product yield.

Applications:

The Discover and the Develop platform technologies can be applied for the de novo development of enzyme reactions or to leverage the initial investment by maximizing the output from an existing enzyme portfolio.

The platform performs in silico predictions in both the synthesis and the degradation direction, and the technologies can be employed for the discovery and development of enzymes for the use in biosynthesis or bioremediation.

References

<https://www.ebi.ac.uk/thornton-srv/transform-miner/>

Internal Reference


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Key Inventors

Dr. Jonathan Tyzack
EMBL EBI

EMBLEM TECHNOLOGY TRANSFER GMBH

 Boxbergring 107
D-69126 Heidelberg
Germany

 Tel.: +49 (0) 6221 363 22 10

 info@embl-em.de

 www.embl-em.de