Short Communication

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Future Microbiology 2020 Accelerated molecular dynamics simulation, functional sequence space clustering and experimentally guided machine learning as an integrated tool for the customization of enzyme performance for defined industrial applications

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Enzymes play an important role in a wide range of industries, such as food and feed, agriculture, personal care, textiles, laundry detergents, fine chemicals and pharmaceuticals. Some examples where enzymes are crucial include cheese manufacture, beer and wine making, baking bread, fruit juice extraction and clarification, leather tanning and more recently in the production of biofuels and biopolymers1,2. Further, due to their high enantio- and regio-selectivity, leading to higher yields of the required enantiomer, enzymes are increasingly used in fine chemical synthesis and in the production of chiral pharmaceutical intermediates and APIs.

The enzymes used for various industrial applications can be harvested from microbial sources or they can be customized for a defined industrial application and overexpressed in heterologous hosts such as bacteria, yeasts and filamentous fungi. This type of enzyme engineering is a powerful way to obtain large amounts of a customized enzyme to replace traditional chemical processes3.

The enormous progress made in recent years in this area is based on new approaches for the screening and identification of novel enzymes, on the development of various protein engineering methods to tailor enzymes with the defined or novel properties, and on the availability of sequence and structural data on a wide range of enzymes that give rise to powerful new machine learning approaches. One recently developed technology making an important contribution to the discovery of novel proteins and engineering of customised enzymes for defined industrial applications involves the application of a proprietary enzyme design platform overcoming key efficiency bottlenecks in statistical structure-dynamics analysis4 and enabling the streamlined functional clustering of protein sequence space. This powerful technique allows the fast and reliable identification and subsequent engineering of hotspots in a protein, resulting in a rapid and inexpensive improvement of enzyme properties, such as chirality, catalytic activity, stability, substrate specificity, stereoselectivity. Further, this technology can apply function to sequences during enzyme discovery, thereby enabling the identification of protein homologues with potentially better properties than the target enzyme and provides outstanding opportunities for the selection and subsequent design of industrial enzymes with the desired properties. This presentation seeks to provide a description of this enzyme design technology in the discovery and design of customized enzymes.

Biography :

Henryk Kalisz obtained his PhD in Biochemistry at Manchester University, having published over 60 papers in reputed scientific journals. He has over 30 years of experience in industrial enzymology and biotechnology. After his PhD, he worked as a post-doctorate at the University of Freiburg, Freiburg, Germany, before taking up a senior scientist role at the National Research Institute (Gesellschaft für Biotechnologische Forschung) in Braunschweig, Germany. He subsequently worked as Head of Biochemistry at Pharmacia, Nerviano, Italy, and as Chief Scientific Officer at Eucodis Bioscience in Vienna, Austria. Since October 2011 he has been applying his expertise in industrial enzymology as a consultant and independent representative to provide scientific and technological advice and assistance to various Biotechnology and Pharmaceuticals organizations.

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