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Tailoring enzymes for defined industrial applications by integrating accelerated molecular dynamics simulation, functional sequence space clustering and experimentally guided machine learning.

Enzymes play an increasingly important role in a wide range of industries, including food and feed, textile, detergent, fine chemicals and pharmaceuticals. 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 plethora of enzymes that give rise to powerful new machine learning approaches. One of the recently developed technologies making an important contribution to the discovery of novel proteins and engineering of tailor-made enzymes for defined industrial applications involves the application of a proprietary enzyme design platform overcoming key efficiency bottlenecks in statistical structure-dynamics analysis 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 highlight the major areas of enzyme application and to provide a description of this enzyme design technology.

Biography

Henryk Kalisz obtained his PhD in Biochemistry at Manchester University and has published over 60 papers in reputed scientific journals. He has over 30 years of experience in industrial enzymology and biotechnology, including as Head of Biochemistry at Pharmacia Italy (Nerviano) 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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