

acib TECHNOLOGY OFFER

In-silico identification of novel enzymes

The present invention uses bioinformatics methods to mine structural databases using three dimensional search templates termed "catalophores". This technology can be applied to find enzymes catalyzing the same reaction, but without sequence similarities.

BACKGROUND

In-silico prediction and identification of enzyme functionalities are used to reduce wet-lab screening costs. However, conventional methods use either the overall sequence identity or specific sequence patterns and usually just find "more of the same". Instead, we have developed a novel computational tool to identify enzymes based on active-site constellation and cavities.

TECHNOLOGY

Generation 1 of our enzyme search platform was able to mine structural databases using 3-D search templates covering the active site configuration of enzymes (published in Nature Communications DOI: 10.1038/ncomms5150).

Generation 2 is a significant improvement of this concept using pre-calculated point-clouds representing physico-chemical properties of the "empty space" in enzyme

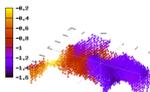
GENERATION 1



3D DESCRIPTORS
PSEUDO CENTERS
AMINO ACID PROPERTIES

REACTION MECHANISM
HIGH SCIENTIFIC INPUT
SEARCH SCRIPT

GENERATION 2



3D CAVITY POINT CLOUD
PHYSICO-CHEMICAL
PROPERTIES OF
„EMPTY SPACE“

SELECT SEARCH
CAVITY

active sites. This allows the identification of alternative enzymes for biocatalytic processes and medical applications without detailed knowledge of the involved reaction mechanism and will even enable cross-reactivity comparisons of e.g. therapeutically relevant inhibitors.

BENEFITS

- 3D-enzyme search (independent of amino acid sequence)
- Automatic cavity point-cloud and property generation
- Ranked hitlist based on multi-dimensional similarity scores
- No knowledge of the involved reaction mechanism required
- Find enzymes not covered by patents (relying on sequence protection) or include them in your patent to make it stronger

innoPhore

innoPhore is a young biotech spin-off from acib GmbH, the Austrian Centre of Industrial Biotechnology and the University of Graz.

Plüddemanngasse 39
A-8010 Graz, Austria
+43 316 873 9118
office@innoPhore.com
http://innoPhore.com



www.acib.at

KEYWORDS:

- enzyme search
- novel enzymes
- catalophore
- enzyme search platform
- innoPhore

INVENTORS:

Christian Gruber
Karl Gruber
Georg Steinkellner

AVAILABLE FOR:

- License agreement
- Collaboration
- Contract research

IPR:

WO2014080005 A1

CONTACT:

Dr. Martin Trinker

ACIB - Austrian Centre of Industrial Biotechnology
Director Business Development
Petersgasse 14/V
8010 Graz
T: +43 316 873 9316
martin.trinker@acib.at