Masterclass "Computational Approaches and In Silico Enzyme Library Design for Applied Biocatalysis"

University of Groningen
Linnaeusborg & Bernoulliborg, Nijenborgh 7, 9747AG Groningen, The Netherlands
Date: July 1-5, 2019

Goal

The course aims to make participants familiar with the use of structural biology and computational tools for engineering the performance of enzymes that are relevant for applied biocatalysis and synthetic biology. The course provides both a theoretical background on computational methods relevant to enzyme engineering (protein crystallography, homology modeling, energy calculations, protein design, smart libraries), and hands-on computer exercises on visualization and analysis of enzymes structures, including docking simulations and enzyme redesign. The theoretical and practical parts are integrated in a few problem-solving modules. Participants will have the opportunity to share their research via short oral presentations, posters, and interactive lectures.

Topics

Protein crystallography and structure analysis
Homology modeling, quantum mechanical modeling
Docking and molecular dynamics simulations (Yasara)
Computational enzyme (re)design (Rosetta, FoldX, FRESCO)
Enzyme engineering supported by web tools (HotspotWizard, CaverWeb, FireProt, PredictSNP, EzymeMiner)
Sequence- and structure-based design of smart libraries
Thermostability and (stereo)selectivity engineering
Industrial examples of enzyme engineering

Tutors and teachers

Dick Janssen, Hein Wijma and Andy-Mark Thunnissen, University of Groningen
Jiri Damborsky, and David Bednar, Masaryk University, Brno
Marc van der Kamp, University of Bristol
Rene de Jong, DSM Delft
Emanuele Monza, Zymvol, Barcelona
t.b.a.

Masterclass coordination

Dick Janssen, Hein Wijma, Marco Fraaije, University of Groningen, The Netherlands
Jiri Damborsky and David Bednar, Masaryk University, Brno, Czech Republic
Sandra Haan & Tamara Hummel, GBB, University of Groningen, The Netherlands

Intended participants

PhD students, post docs and other researchers skilled in biochemistry who want to become familiar with structure-based and computational approaches in Enzyme Engineering. Partners of the H2020 ES-Cat, Oxytrain, Robox and other EU collaborative projects and training networks are offered priority reduced fee registration. Note: participants are offered the opportunity to share &discuss their research via posters and oral presentations.

Info and registration

Details at: https://www.rug.nl/research/gbb/education/masterclasses/computational/
Questions to: mccomputational@rug.nl.