Masterclass "Computational Approaches for Discovery and Engineering of Enzymes for Biocatalysis and Synthetic Biology"

July 1-5, 2019
University of Groningen,
Linnaeusborg & Bernoulliborg, Nijenborgh 9 and 7, 9747 AG Groningen, The Netherlands

Outline

- 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.
- Provides both a theoretical background on computational methods relevant to enzyme engineering (protein crystallography, homology modeling, energy calculations, protein design, smart libraries).
- Hands-on computer exercises on the analysis of enzymes structures, including model building, docking simulations, use of web tools for library construction and enzyme redesign.
- Also suitable for non-experts in computational techniques.
- Participants will have the opportunity to share their research via short oral presentations, posters, and interactive lectures.

Tutors and teachers

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

- ✓ Participant talks

Day 1, Monday July 1, 2019	Day 2, Tuesday July 2, 2019	Day 3, Wednesday July 3, 2019	Day 4, Thursday July 4, 2019	Day 5, Friday July 5, 2019
8.30-9.15 Registration 9.15 - 9.45 Janssen Opening, introduction	9.00 - 9.45 Wijma Energy functions and docking simulations	9.00 - 9.45 Damborsky Engineering tunnels & ligand transport – concepts and tools	9.00 - 9.45 Bednar Gene mining & engineering stability, solubility	9.00 - 9.45 de Jong Enzyme engineering for industrial biotech
10.00-10.45 Thunnissen X-ray crystallography	10.00-10.45 Wijma Energy functions, search algorithms and computational design	10.00-10.45 Damborsky Engineering tunnels & ligand transport – case studies	10.00-10.45 Bednar Webtools: gene mining & engineering stability, solubility	10.00-10.45 de Jong Computional industrial enzyme redesign
11.00 -11.45 Thunnissen X-ray structures	11.00 -11.45 Monza Computer-aided laccase engineering	11.00 -11.45 Tba, Participant talks	11.00 -11.45 vd Kamp QM modeling of enzyme reactions	11.00 -11.45 Wijma/Oliveira/Ramirez Comp practical: computer simulations, inspection
12.00 Wijma Energy functions and MD simulations	12.00-12.45 Tba, Participant talks	12.00-12.45 Tba, Participant talks	12.00-12.45 vd Kamp Multiscale modeling	12.00 -12.45 Wijma/Oliveira/Ramirez Comp practical: computer simulations, inspection
12.45-14.00 lunch	12.45-14.00 lunch	12.45-14.00 lunch	12.45-14.00 lunch	12.45-14.00 lunch
14.00-17.30 Thunnissen/Rozeboom Comp practical: X-ray, model building, inspection	14.00-17.30 Wijma/Oliveira/Bombino Comp practical: Linux, modeling, docking simulations	14.00-17.30 Damborsky/Bednar Computer practical: web tools for protein engineering	14.00-17.30 Wijma/Oliveira/Ramirez Practical: Rosetta computational redesign	14.00-16.00 Wijma/Oliveira/Ramirez Comp practical: computer simulations, inspection
Dinner	Dinner	Dinner on your own	Dinner	16.00 End of course