PhD position: Molecular dynamics simulations and modification of multi enzyme complexes

Project: BMBF Multizym 2020+
Project leader: Dr. Uwe Jandt
Project term: 2013 – 2017
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Description:
Multi-step enzyme-catalyzed reactions in vitro often suffer from increasing inhibition of enzymes by products or intermediates, molecular crowding and diffusive loss of intermediates. Natural reaction cascades in living cells cope with this problem by establishing temporary or persisting reaction channels within multiple enzymes or enzyme complexes, a process called metabolon or metabolic channeling, respectively. The molecular fundamentals of metabolic channeling in large enzyme complexes have not yet been systematically elucidated. A typical example is the eukaryotic pyruvate dehydrogenase complex (PDC), which catalyzes the irreversible reaction from pyruvate to Acetyl-CoA and thereby links glycolysis to the TCA cycle and also the fatty acid synthesis pathway (Fig. 1).

The candidate will employ Molecular Dynamics (MD) simulations to characterize the structural and mechanistic aspects of the metabolic channeling in multi-enzyme complexes such as the PDC and provide information for targeted protein design, process design and multi-scale modeling technologies for the ultimate common goal of enzyme engineering and design of efficient cell-free enzymatic reaction cascades (Fig. 2) [3].

Qualifications and experience:
Applicants should have an MSc or diploma degree in electrical engineering, bioinformatics, life sciences, biophysics, or computer sciences. Programming skills, knowledge of protein structure and function and experience in macromolecular modeling and dynamics simulation of biological systems are desired.

We offer:
• Multidisciplinary research institute in the field of bioprocess and biosystems engineering.
• Team of highly qualified ambitious co-workers.
• Excellent scientific and cultural infrastructure of Hamburg metropolis.
• Full time payment according to the German salary rules for the public service (TVöD).
• Total appointment time for PhD thesis: 3 years.

Please send your application including curriculum vitae, letter of motivation, diploma certificates (Master / Bachelor degree), and the contact details of a potential reference to Dr. Uwe Jandt (English/German).

References:

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