CeNT CENTRE OF NEW TECHNOLOGIES

UNIVERSITY OF WARSAW

invites to a seminar by

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Centre of New Technologies UW

Design of new protein structures

8th June 2017 at 12:00 p.m.

Venue: Centre of New Technologies, Banacha 2C,
Lecture Hall 0142 (ground floor)

Host: Prof. Joanna Kargul

Protein design, also named inverse folding, is a procedure for computing sequences that will fold to a given target structure. The computational design procedures are used to modify known proteins (redesign), but also to create new structures never seen before in nature (*de novo* design). The successful *de novo* design of proteins with sequences and structures unrelated to those in nature has important implications. The existence of such artificial proteins suggests that evolution has explored only a tiny region of the sequence space that is accessible to proteins. The aim of our project is to design *de novo* a highly-regular protein structure that will contain a secondary structure element termed pi-helix. In contrast to the abundant alpha-helices and beta-sheets, pi-helices are much less frequent in protein structures, mostly due to their instability. The presentation will be focused on the basic concepts of protein design, its application, and the development of a computational pipeline for design of precisely defined pi-helical structures. The pipeline allows to calculate the starting target structures with the aid of the parametric equations and to design tens of thousands of sequences compatible with these structures. Given the fact that only few of those sequences can be tested experimentally, it is essential to narrow down the list of possibilities. To select the most promising candidates, which are likely to fold spontaneously to stable structures, we use molecular dynamics and structure folding simulations. The final goal of the project will be to obtain an NMR or X-ray structure of designed pi-helical protein.