CeNT CENTRE OF NEW TECHNOLOGIES

UNIVERSITY OF WARSAW

invites to a seminar by

prof. Janusz M. Bujnicki,
International Institute of Molecular and Cell Biology;
Adam Mickiewicz University

Computational modeling of macromolecular complexes

January 19 2017 at 1:00 p.m.

at the Centre of New Technologies, Banacha 2c,
room 0142 (ground floor)

Abstract: Macromolecular complexes play fundamental roles in many biological processes, such as the regulation of gene expression, RNA splicing and protein synthesis. Structures of some of these complexes have been experimentally determined, providing insight into mechanisms of their biological activities. However, for a great majority of large biological machines, high-resolution structures are only available for some isolated components, often accompanied with low-resolution information about the overall shape (e.g. from cryo-EM or SAXS) or about the proximities and interactions of these components (e.g. from chemical cross-linking experiments). Given the scarcity of experimentally determined structures, computational techniques can be used to integrate heterogeneous pieces of information, guide structure elucidation and subsequently determine the mechanisms of action and interactions between the components.

I will present methods for computational modeling of protein-protein and protein-nucleic acid complexes developed in our laboratory, in particular PyRy3D, a program that predicts structures based on low-resolution experimental data and enables the construction of models even for very large complexes with components of unknown or disordered 3D structure. Our software is available at http://genesilico.pl.