

FEBS Advanced Course Ligand-binding Theory and Practice July 3 - 10, 2016 Academy and University Center Nove Hrady Czech Republic Intermolecular interactions – between or among proteins, nucleic acids, or small molecules – underlie virtually every aspect of biology. Quantitative analysis of these interactions to determine their affinity, specificity, stoichiometry, cooperativity (allostery), and kinetics is a required first step toward understanding their biological roles. Recent developments in a range of new analytical methods have made direct quantitative study of macromolecular interactions readily accessible even to those with limited background in ligand-binding theory. Although the theory is rooted in the most elementary principles of general chemistry, it is very often applied poorly, leading to incorrect or ambiguous results, many of which have found their way into the literature over the years, limiting pur understanding of interactions in important biomolecular systems.

This course will provide basic training in the principles of ligand-binding theory, and will offer students a chance to analyse their own macromolecular interaction systems using the contemporary advanced methods of surface plasmon resonance SPR, isothermal titration calorimetry ITC, UV-vis and fluorescence spectroscopies, and microscale thermophoresis, guided by lecturers and tutors who are experts in the design, execution, and analysis of these experiments. Students will also gain exposure to contemporary experimental ligand-binding methods that are not represented among the practicals, including NMR, mass spectrometry, analytical ultracentrifugation AUC, vibrational spectroscopies, and others, through presentations by lecturers who are expert in each method. Besides ligand binding per se, a second unifying theme of the lectures will be allostery, also known as cooperativity. Nobelist Jacques Monod is said to have regarded allostery as life's second secret, and study of allosteric mechanisms is widely regarded as the most important contemporary application of ligand-binding studies. Among the lecturers on allostery will be experts who will debate our current understanding of hemoglobin, the most well-known biological manifestation of cooperative ligand binding. The course is aimed for practitioners of ligand binding at the graduate or early postdoctoral level, although our experience indicates that even more advanced practitioners will also increase their competency, enabling them to disseminate an accurate understanding of this critical topic. Basic training in the fundaments of ligand-binding theory will open the course, to enable all students to acquire the principles that can support their experiments and leverage the subsequent lecture program of expert speakers. This training will also equip students with the skills to critically evaluate published binding data in any molecular system. The first half-day will include lectures, group discussion, and problem-solving exercises in a first seminar directed by Prof. Jannette Carey, and computational analysis, simulation, and data analysis in a workshop directed by Prof. Wei-Feng Xue. The course will conclude with a workshop on global analysis of each student's own ligand binding results in a seminar directed by Prof. Xue.

Organizers

Jannette Carey, Ph.D.: Professor Carey has over twenty-five years' experience in applying and teaching ligand-binding theory with graduate, post-graduate, and advanced undergraduate students at Princeton University, New Jersey, USA. She She has developed a simple treatment that is proven to reach students with a wide range of backgrounds, giving them the skills to design and analyze ligand-binding experiments. She holds a prestigious position as visiting scientist of the Academy of Sciences of the Czech Republic at Nove Hrady, and has participated since 2006 as a speaker and/or tutor in the FEBS practical and lecture course, Advanced methods in macromolecular crystallography. She initiated and organized the first FEBS practical and lecture course devoted to ligand binding in 2014. As in 2014, she will act as lecturer for the opening lessons on ligand-binding theory, and as a general tutor overseeing all the laboratory practicals of the course. Additionally, she will give a general lecture about ligand-binding methods.

Wei-Feng Xue, Ph.D.: Professor Xue is an Associate Professor (Senior lecturer in Chemical Biology) at the University of Kent. He is an expert in all aspects of ligand-binding theory and applications, particularly with the experimental and computational methods to be offered on this course. He has been a collaborator of Prof. Carey for over fifteen years. As in 2014, he will act as tutor for the computational sessions held on the first and last lecture days of the course, as tutor for the SPR practical, and as a general tutor overseeing all the laboratory practicals of the course together with Prof. Carey.

Rüdiger Ettrich, Ph.D.: Professor Ettrich heads the Center for Nanobiology and Structural Biology in Nove Hrady. His research is focused on the relationship between structure and function of proteins, dynamic changes related to functional processes, and the mutual interaction of cofactors and subunits in protein complexes. The research approach uses diverse research methods with a synthesis of theory and experiment. Rüdiger Ettrich is coordinating several multidisciplinary research projects and has an extensive network of international collaborators. He is a long-time collaborator of the coorganizer of this course, Prof. Jannette Carey from Princeton University. His research laboratories will accommodate the course practicals using his instruments for ITC, SPR, and UV-vis and fluorescence spectroscopies. Together with Prof. Carey and Prof. Xue he organized the first FEBS practical and lecture course devoted to ligand binding in 2014.