Preface

This volume comprises papers presented at the 2014 edition of the "Crystallography of Molecular Biology" series. These courses are part of a wide-ranging set of crystallography courses held since 1974 in the hilltop town of Erice, Italy, at the Ettore Majorana Foundation and Centre for Scientific Culture. This series of courses is renowned for bringing leaders in the fields of macromolecular crystallography and biomedicine together with highly motivated students in a warm and informal atmosphere, which encourages a high level of interactions. Lecturers were chosen from world leaders in the fields of structure-based drug design, biochemistry, biophysics, bioinformatics, computational chemistry, and structural biology, and all made great efforts to present cutting-edge science at a level accessible to participants with limited experience. Most presented two lectures, one focused on methodology and another illustrating the structural insights that can be obtained using their methods.

The course included plenary lectures, as well as talks chosen from poster abstracts submitted by participants. Lectures covered a wide-range of topics including targeting protein-protein interactions, structure determination of G-protein coupled receptors and other membrane proteins, evolution of biopharmaceuticals, understanding of epigenetic processes, and targeting kinases and ribosomes for drug development. Protein-ligand interactions were discussed from multiple perspectives; from the use of high-resolution protein structures to demonstrate the importance of water molecules and protons in protein-ligand interactions to the detailed thermodynamic and kinetic studies that can be performed to fully understand the biochemistry of the interactions. Different approaches to drug discovery and development were highlighted by several talks, including drug discovery and design in pharmaceutical industries and the use of protein engineering and crystallographic fragment screening. Several talks addressed the problem of drug resistance and the steps that can be taken to prevent or minimize it. Discussion was not solely limited to experimental approaches: novel computational techniques for structural bioinformatics, lead generation, prediction of protein aggregation, and

the use of molecular modelling and data mining to improve drug discovery success rate were also described. The growing importance and evolving roles of structural databases, essential to ensure all data are properly archived and accessible to the public, were also discussed.

The real organizational work of the course was done by Paola Spadon and Annalisa Guerri who, between them, found most of the funding, corresponded with and coordinated the participant selection and together with the team of 'orange scarves' (Fabio Nicoli, Giovanna Avella, Julia Magliozzo, Giancarlo Tria, and Francesca Vallese) created a warm and welcoming environment in which students were free to engage in scientific discussion with their peers and scientific experts. Erin Bolstad played an essential role, organizing all the computing facilities necessary to conduct tutorials and demonstrations, and providing, together with Fred Boyle, Gianni Grassi, and the Ettore Majorana Center staff, superb IT support. The scientific organizers were Eddy Arnold, Richard Pauptit, Giovanna Scapin, and Robert Stroud. Sir Tom Blundell has been the Director of the International School for Crystallography since 1982.

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