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In references *Topics in Current Chemistry* is abbreviated Top Curr Chem and is cited as a journal.

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ISBN 978-3-540-49079-1 e-ISBN 978-3-540-49080-7
DOI 10.1007/978-3-540-49080-7

Topics in Current Chemistry ISSN 0340-1022

Library of Congress Control Number: 2007942195

Cover design: WMXDesign GmbH, Heidelberg
Typesetting and Production: le-tex publishing services oHG, Leipzig

Printed on acid-free paper

9 8 7 6 5 4 3 2 1 0

springer.com

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Preface

Specific binding of a ligand to a receptor is a key step in a variety of biological processes, such as immune reactions, enzyme cascades, or intracellular transport processes. The ligand–receptor terminology implies that the receptor molecule is significantly larger than the ligand, and the term "bioactive conformation" usually characterizes the conformation of a ligand when it is bound to a receptor. In a more general sense, bioactive conformation applies to any molecule in a biologically relevant bound state regardless of size considerations. Most of the contributions to this book address ligands that are much smaller than their receptors.

X-ray crystallography and high resolution NMR spectroscopy are the two main experimental techniques used to study bioactive conformations. Therefore, the two volumes of this book cover approaches that use either of the two techniques, or a combination thereof. The combination of X-ray crystallography and NMR spectroscopy is particularly useful when a crystal structure of a receptor protein, but not of the receptor protein–ligand complex, is available. A number of experimental techniques to analyze the bioactive conformation of a ligand with NMR are based on the observation of the resonance signals of the free ligand that is in exchange with the bound ligand. Several chapters focus on such approaches that range from "classical" transferred NOE experiments, to transferred dipolar couplings, to STD (saturation transfer difference) NMR techniques. In cases where tight binding in the sub-nanomolar range prevents the analysis of the bioactive conformation via free ligand signals, the ligand–protein complex has to be analyzed with protein NMR-based techniques or by crystallography. Since this area has been the subject of many reviews and monographs it will not be covered here in particular detail. As a unifying theme, all contributions target the question of how molecular recognition of biologically active molecules is achieved on the atomic scale. Depending on the research topic the results from these studies have a strong impact not only in basic research but also in several fields of application ranging from pharmaceutical applications to the use of biomolecules as, for example, cryoprotectants.

Almost all contributions to the two volumes highlight the fact that ligand–protein complexes cannot be treated as static ensembles. On both sides, the ligand and the receptor side, dynamic processes contribute to the molecular recognition. In this sense it is hoped that these two volumes of *Bioactive Confor-*

mation will sensitize us for the need to invent and develop more experimental techniques to study the dynamic aspects of bioactive conformations.

Lübeck, December 2007 Thomas Peters

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Volume Editor: Peters, T.
ISBN: 978-3-540-49077-7