

Protein–Ligand Interactions

Methods and Applications

Edited by

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Molecular recognition and binding of ligands (atoms, ions, and molecules) by proteins with high sensitivity and selectivity is of central importance to essentially all biomolecular processes and of key importance for the basic and applied sciences. In *Protein–Ligand Interactions: Methods and Applications*, leading experts with hands-on experience describe in detail a broad selection of established and emerging techniques for studying the interaction between proteins and ligands, including bulk biochemical techniques, structure analysis, spectroscopy, single-molecule studies, and theoretical/computational tools. Among the highlights are surface plasmon resonance (SPR) and reflectometric biosensor approaches, high-throughput screening with confocal optics microscopy, single molecule fluorescence and fluorescence correlation spectroscopy (FCS), atomic force microscopy (AFM), crystallography of reaction intermediates, and time-resolved X-ray crystallography. The protocols follow the successful *Methods in Molecular Biology*™ series format, each offering step-by-step laboratory instructions, an introduction outlining the principle behind the technique, lists of the necessary equipment and reagents, and tips on troubleshooting and avoiding known pitfalls.

Cutting-edge and highly practical, *Protein–Ligand Interactions: Methods and Applications* offers novice and expert researchers alike a broad selection of powerful and widely applicable techniques that can be used to efficiently and successfully solve the task of characterizing protein–ligand interactions.

FEATURES

- Readily reproducible techniques for studying protein–ligand interactions
- Broad selection of established, novel, and emerging methodologies
- Emphasis on novel techniques as well as on recent advances in classical methods
- Discussion of theoretical issues relevant to each technique
- Details on the use of AFM and fluorescence with single-molecule sensitivity
- Surface plasmon resonance and reflectometric biosensor approaches
- Crystallography of reaction intermediates and time-resolved X-ray crystallography
- High-throughput screening with confocal optics microscopy

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Isothermal Titration Calorimetry. Direct Optical Detection of Protein–Ligand Interactions. Label-Free Detection of Protein–Ligand Interactions by the Quartz Crystal Microbalance. Measurement of Solvent Accessibility at Protein–Protein Interfaces. Hydrophobic Interaction Chromatography: Harnessing Multivalent Protein–Surface Interactions for Purification Procedures. Sedimentation Velocity Method in the Analytical Ultracentrifuge for the Study of Protein–Protein Interactions. Protein–Ligand Interaction Probed by Time-Resolved Crystallography. X-Ray Crystallography of Protein–Ligand Interactions. Combined Use of XAFS and Crystallography for Studying Protein–Ligand Interactions in Metalloproteins. NMR Studies of Protein–Ligand Interactions. Probing Heme Protein–Ligand Interactions by UV/Visible Absorption Spectroscopy. Ultrafast Time-Resolved IR Studies of Protein–Ligand Interactions. Monitoring Protein–Ligand Interactions by Time-Resolved FTIR Difference Spectroscopy. Proteins in Motion: Resonance Raman Spectroscopy as a Probe of Functional Intermediates. Fluorescence Polarization/Anisotropy Approaches to Study Protein–Ligand Interactions: Effects of Errors and Uncertainties. Ligand Binding

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