Biophysical Techniques in Drug Discovery

Angeles Canales Universidad Complutense de Madrid, Spain

Synopsis
Biophysical techniques are used in many key stages of the drug discovery process including screening of new ligands for a certain receptor, characterisation of a drug mechanism and validation of data from biochemical and cellular assays. This title, with contributions from both academia and industry, brings together the different elements of biophysical techniques within drug discovery in a single volume. Topics covered include the characterisation of integral membrane proteins and their interactions with drugs, G protein-coupled receptors and important developments in the field such as improvement in electron microscopy resolution.

Brief Contents
- Impact and Evolution of Biophysics in Medicinal Chemistry
- Ligand-Detected NMR Methods in Drug Discovery
- Receptor based NMR techniques in Drug Discovery
- Mass Spectrometry in Biophysics: from High Throughput Screening to Structural Biology
- Characterization of Pharmaceutical Solids Combining NMR, X-ray Diffraction and Computer Modelling
- Surface Plasmon Resonance for Identifying and Characterising Small Molecule Ligands
Computational Tools for Chemical Biology

Sonsoles Martín-Santamaría Centro de Investigaciones Biológicas CIB-CSIC, Spain

Synopsis
The field of computational chemical biology involves utilizing the latest techniques to visualise and manipulate processes within living cells. The rapid development of efficient computational tools has allowed researchers to tackle biological problems and to predict, analyse and monitor, at an atomic level, molecular recognition processes. This book, with contributions from internationally renowned experts as well as new leaders in the field, offers a fresh perspective on how computational tools can aid the chemical biology research community.

Brief Contents
- Computational chemistry and molecular modelling basis
- Molecular graphics and modelling tools in chemical biology
- Development of MM and QM/MM molecular dynamics algorithms for the computation of biological systems
- Molecular dynamics and coarse-grained simulations: where we are and where we can go
- Molecular and Cellular Modelling: simulations of biomolecular interactions
- Computational structural biology
- Molecular modelling of nucleic acids
- Computational enzymology: modelling biological catalysts
Drug Discovery for Leishmaniasis

Luis Rivas Centro de Investigaciones Biológicas (CSIC), Spain
Carmen Gil Centro de Investigaciones Biológicas (CSIC), Spain

Synopsis
From a human health perspective, leishmaniasis is among the most important protozoan diseases, superseded only by malaria. Between 10 and 12 million people are affected by the disease and with no known vaccine, the development of new drugs is urgently required. This volume provides a perspective of current treatments and their challenges as well as discussing emerging strategies and methodologies that will drive new drug development for this ‘neglected’ disease.

Brief Contents
- Appraisal of Leishmaniasis chemotherapy, current status and pipeline strategies
- Methodologies and medicinal chemistry strategies to discover and develop new treatments
- The quest for Achille´s heel of Leishmania: Singular targets as new avenues for drug development

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Gas Sensing in Cells
Shigetoshi Aono CIMoS, Japan

Synopsis
Gas sensor proteins that detect specific gaseous molecules are involved in many biological regulatory and detoxification systems. This book provides the first comprehensive overview of gas sensing in living cells and describes a wide spectrum of proteins that produce, sense or use gas molecules in both prokaryotic and eukaryotic cells. This book will be particularly interesting to postgraduates and researchers in biochemistry, molecular biology and metallobiology.

Brief Contents
- Overview of Gas Sensing Systems
- Haem-Based Sensors of Nitric Oxide
- Haem-Based Sensors of Dioxigen
- Haem-Based Sensors of Carbon Monoxide
- Iron-Sulfur Cluster-Based Sensors
- Non-Haem Iron-Based Sensors of Reactive Oxygen and Nitrogen Species
- Mammalian O2 Sensing and Signalling
- Plant Ethylene Sensing and Signalling
- Subject Index

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Dynamical Astrochemistry

David A Williams University College London, UK
Thomas W Hartquist University of Leeds, UK
Jonathan C Rawlings University College London, UK
C Cecchi-Pestellini Università degli Studi di Palermo, Italy
Serena Viti University College London, UK

Synopsis
Astrochemistry is a well-established interdisciplinary subject. Existing astrochemical books normally describe the subject in terms of chemistry in static or slowly-varying astronomical situations but the most significant astronomical regions are those in which the physical conditions change on timescales that are comparable to or shorter than chemical timescales. This is the first book specifically devoted to the astrochemistry of dynamically evolving astronomical regions. It provides a comprehensive description of this important area of science, stressing in particular the methods that have been developed for specific purposes. It will be of interest to researchers in astrochemistry, including both chemists and physicists and could form the basis of a postgraduate course for research students in chemistry and physics.

Brief Contents
- Chemistry and Dynamics in the Interstellar Medium
- Shocks and Turbulence and Their Effects on Chemistry
- Non Thermal Chemistry in the Interstellar Medium
- Infall: gas dynamics under gravity
- Stellar Jets and Outflows
- Outflows and Explosions of Evolved Stars
- Conclusions: where do we go from here?