

Contents

Application of Computational Methods to the Design of Fatty Acid Amide Hydrolase (FAAH) Inhibitors Based on a Carbamic Template Structure

ALESSIO LODOLA, SILVIA RIVARA, AND MARCO MOR

I. Introduction	2
II. Ligand-Based Drug Design	5
III. Structure-Based Drug Design	11
IV. Recent Advances	21
References	22

Recent Theoretical and Computational Advances for Modeling Protein-Ligand Binding Affinities

EMILIO GALICCHIO AND RONALD M. LEVY

I. Introduction	28
II. Theory of Noncovalent Binding	30
III. Computational Methods	53
IV. Conclusions	73
References	74

Hybrid Schemes Based on Quantum Mechanics/Molecular Mechanics Simulations: Goals to Success, Problems, and Perspectives

SILVIA FERRER, JAVIER RUIZ-PERNÍA, SERGIO MARTÍ, VICENT MOLINER, IÑAKI TUÑÓN,
JUAN BERTRÁN, AND JUAN ANDRÉS

I. Introduction: State of Art	83
II. Potential of Mean Force/Free-Energy Calculations	97
III. Applications	98
IV. Conclusions and Outlook	120
References	129

Exploring Membrane and Protein Dynamics with Dissipative Particle Dynamics

GERNOT GUIGAS, DIANA MOROZOVA, AND MATTHIAS WEISS

I. Introduction.....	144
II. Setting Up DPD Simulations.....	145
III. Investigating Structure and Dynamics of Membranes with DPD.....	162
References	179

Coarse-Grained Representation of Protein Flexibility. Foundations, Successes, and Shortcomings

MODESTO OROZCO, LAURA ORELLANA, ADAM HOSPITAL, ATHI N. NAGANATHAN,
AGUSTÍ EMPERADOR, OLIVER CARRILLO, AND J. L. GELPI

I. Introduction.....	184
II. Coarse-Grained Potentials	188
III. Sampling Techniques.....	200
IV. Conclusions	210
References	212

Recent Advances in the Molecular Modeling of Estrogen Receptor-Mediated Toxicity

IVANKA TSAKOVSKA, ILZA PAJEVA, PETKO ALOV, AND ANDREW WORTH

I. Introduction.....	218
II. Structural Studies of the Estrogen Receptor and Its Ligands	220
III. Molecular Modeling Approaches to Investigate Estrogen Receptor-Mediated Toxicological Effects	228
IV. Molecular Modeling of Estrogen Receptor-Mediated Toxicological Effects: Case Studies.....	234
V. Conclusions	245
References	246

Multiscale Computational Methods for Mapping Conformational Ensembles of G-Protein-Coupled Receptors

NAGARAJAN VAIDEHI AND SUPRIYO BHATTACHARYA

I. Introduction	254
II. Conformational Flexibility in GPCRs	256
III. Computational Approaches for Studying Conformational Ensembles of GPCRs	261
IV. Activation Mechanism of GPCRs	268
V. Concluding Remarks	274
References	275

Advances in Implicit Models of Water Solvent to Compute Conformational Free Energy and Molecular Dynamics of Proteins at Constant pH

YURY N. VOROBJEV

I. Introduction	282
II. Formulation of General Implicit Solvent Model for Calculating Conformational Free Energy	283
III. Continuum Solvent Models	286
IV. Protein Ionization	302
V. Examples of Simulations with Implicit Solvent Models	308
References	314
AUTHOR INDEX	323
SUBJECT INDEX	341