Contents

1 **Hybrid QM/MM Methods: Treating Electronic Phenomena in Very Large Molecular Systems** 1
Antonio Monari and Xavier Assfeld

2 **Structure, Thermodynamics and Energetics of Drug-DNA Interactions: Computer Modeling and Experiment** 21
Maxim P. Evstigneev and Anna V. Shestopalova

3 **Formation of DNA Lesions, its Prevention and Repair** 59
Nihar R. Jena, Neha Agnihotri and Phool C. Mishra

4 **DNA Dependent DNA Polymerases as Targets for Low-Weight Molecular Inhibitors: State of Art and Prospects of Rational Design** 95
Alexey Yu. Nyporko

5 **Molecular Structures, Relative Stability, and Proton Affinities of Nucleotides: Broad View and Novel Findings** 137
Tetiana A. Zubatiuk, Gennady V. Palamarchuk, Oleg V. Shishkin, Leonid Gorb and Jerzy Leszczynski

6 **Quantum Chemical Approaches in Modeling the Structure of DNA Quadruplexes and Their Interaction with Metal Ions and Small Molecules** 181
Mykola Ilchenko and Igor Dubey

7 **Density Functional Theory Calculations of Enzyme–Inhibitor Interactions in Medicinal Chemistry and Drug Design** 207
Alexander B. Rozhenko

8 Molecular Dynamics Simulations of Lipid Bilayers with Incorporated Peptides 241
Milan Melicherčík, Tibor Hianik and Ján Urban

9 Polyphenol Glycosides as Potential Remedies in Kidney Stones Therapy. Experimental Research Supported by Computational Studies 271
D. Toczek, E. Klepacz, S. Roszak and R. Gancarz

10 Quantum-Chemical Investigation of Epoxidic Compounds Transformation. Application for *In Vitro* and *In Vivo* Processes Modeling 295
Sergiy Okovytyy

11 Computational Toxicology in Drug Discovery: Opportunities and Limitations 325
Alexey Zakharov and Alexey Lagunin

12 Consensus Drug Design Using It Microcosm 369
Pavel M. Vassiliev, Alexander A. Spasov, Vadim A. Kosolapov, Aida F. Kucheryavenko, Nataliya A. Gurova and Vera A. Anisimova

13 Continuous Molecular Fields Approach Applied to Structure-Activity Modeling 433
Igor I. Baskin and Nelly I. Zhokhova

14 Quantitative Structure-Property Relationship Analysis of Drugs' Pharmacokinetics Within the Framework of Biopharmaceutics Classification System Using Simplex Representation of Molecular Structure 461
N. Ya. Golovenko, I. Yu. Borisyuk, M. A. Kulinskiy, P. G. Polishchuk, E. N. Muratov and V. E. Kuz'min

15 (How to) Profit from Molecular Dynamics-based Ensemble Docking 501
Susanne von Grafenstein, Julian E. Fuchs and Klaus R. Liedl

16 Cheminformatics: At the Crossroad of Eras 539
Denis Fourches

Index 547

http://www.springer.com/978-94-017-9256-1

Application of Computational Techniques in Pharmacy and Medicine

Gorb, L.; Kuz'min, V.; Muratov, E. (Eds.)

2014, XIII, 550 p. 172 illus., 80 illus. in color., Hardcover
ISBN: 978-94-017-9256-1