1. Record Nr. UNINA9910451218003321

Autore	Day Lincoln H. <1928, >
Titolo	The future of low-birthrate populations / / Lincoln H. Day
Pubbl/distr/stampa	London ; ; New York : , : Routledge, , 1995
ISBN	1-134-79909-8 0-585-45342-X 1-280-32099-0 9786610320998 0-203-43354-8
Descrizione fisica	1 online resource (xviii, 186 pages) : illustrations
Disciplina	304.6/2
Soggetti	Fertility, Human - Europe Demographic transition - Europe Electronic books. Europe Population policy
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Book Cover; Title; Contents; List of figures; List of tables; Foreword; Preface; THE DEMOGRAPHIC SITUATION; THE FUTURE OF FERTILITY AND MORTALITY; THE CHALLENGE OF NUMERICAL DECLINE AND OLDER AGE STRUCTURE: PART 1. FINANCES AND THE PROVISION OF CARE; THE CHALLENGE OF NUMERICAL DECLINE AND OLDER AGE STRUCTURE: PART 2. HOUSEHOLDS, LABOR FORCE, ECONOMIC CONDITIONS AND BEHAVIOR; POLICY ALTERNATIVES: DEMOGRAPHIC; SOME COMPENSATIONS IN THE TREND TOWARD OLDER AGE STRUCTURES AND NUMERICAL DECLINES; POLICY ALTERNATIVES: NONDEMOGRAPHIC; CONCLUSION; Index;
Sommario/riassunto	Lincoln Day assesses the demographic situation, the likely policy alternatives, the significance of future changes in fertility and mortality rates and analyses the likely losses and gains attendant upon an ageing, dwindling people.

2. Record Nr. UNINA9910298644203321

Titolo	Application of Computational Techniques in Pharmacy and Medicine / / edited by Leonid Gorb, Victor Kuz'min, Eugene Muratov
Pubbl/distr/stampa	Dordrecht : , : Springer Netherlands : , : Imprint : Springer, , 2014
ISBN	94-017-9257-7
Edizione	[1st ed. 2014.]
Descrizione fisica	1 online resource (556 p.)
Collana	Challenges and Advances in Computational Chemistry and Physics, , 2542-4491 ; ; 17
Disciplina	054 541.2 570285 610
Soggetti	Chemistry, Physical and theoretical Pharmaceutical chemistry Pharmacy Bioinformatics Medicine Theoretical and Computational Chemistry Medicinal Chemistry Biomedicine, general
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
Nota di contenuto	1 Hybrid QM/MM Methods: Treating Electronic Phenomena in Very Large Molecular Systems -- 2 Structure, Thermodynamics and Energetics of Drug-DNA Interactions: Computer Modeling and Experiment -- 3 Formation of DNA Lesions, Its Prevention and Repair -- 4 DNA dependent DNA Polymerases as Targets for Low-Weight Molecular Inhibitors: State of Art and Prospects of Rational Design -- 5 Molecular structures, relative stability, and proton anities of nucleotides: Broad view and novel findings -- 6 Quantum Chemical Approaches in Modeling the Structure of Quadruplex DNA and Its Interaction with Metal Ions and Small Molecules -- 7 Density Functional Theory Calculations of Enzyme-Inhibitor Interactions in Medicinal

Chemistry and Drug Design -- 8 Molecular Dynamics Simulations of Lipid Bilayers with Incorporated Peptides -- 9 Polyphenol Glycosides as Potential Remedies in Kidney Stones Therapy. Experimental Research Supported by Computational Studies -- 10 Quantum-Chemical Investigation of Epoxidic Compounds Transformation. Application for In Vitro and In Vivo Processes Modeling -- 11 Computational Toxicology in Drug Discovery: opportunities and limitations -- 12 Consensus Drug Design Using it Microcosm -- 13 Continuous Molecular Fields Approach Applied to Structure-Activity Modeling -- 14 Quantitative Structure-Pharmacokinetic Relationships of Drugs within the Framework of Biopharmaceutics Classification System by Using Simplex Representation of Molecular Structure -- 15 (How to) Profit from Molecular Dynamics-based Ensemble Docking -- 16 Cheminformatics on Crossroad of Eras.

Sommario/riassunto

The current volume provides both fundamental and detailed information about the computational and computational-experimental studies which improve our knowledge of how leaving matter functions. It also covers research areas related to structures and properties of drugs (including the calculation and the design of new ones), and the development of completely new ways of treating numerical diseases. Whenever it is possible, the interplay between theory and experiment is emphasized. The book features computational techniques such as quantum-chemical and molecular dynamic approaches supplemented by a discussion on quantitative structure–activity relationships. The initial chapters describe the state-of-the art computational approaches for molecular biology, molecular pharmacy, and molecular medicine performed with the use of pure quantum-chemical techniques. The central part of the book illustrates the status of computational techniques that utilize hybrid, so called QM/MM approximations. In addition, the results of the QSAR studies, which now are the most popular in predicting drugs' efficiency, are discussed. The last chapter reveals the current state of chemoinformatics and discusses new problems and experimental perspectives related to both chemical and biological characteristics of molecules.