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Molecular switches and logic gates for information processing, the bottom-up strategy: from silicon to carbon, from molecules to supramolecules 181

M.F.Budyka

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The chemistry of molecular logic gates is a new science, which arose in the late 20th century at the intersection of chemistry, physics, electronics and logical algebra. The molecular gates differ from the currently used semiconductor elements by small size, multifunctional nature and variability of input and output signals. The review considers molecular gate functioning mechanisms and design algorithms based on the compound structure and properties. The criteria to be satisfied by a molecular system to function as a molecular logic gate are given. The experimental data on the modelling of functions of logic gates at the molecular level are critically analyzed. Particular attention is given to photonic molecular gates, which can operate without any connecting wires or added chemicals, unlike molecular gates with chemical inputs or semiconductor gates. The problems of further development of molecular logic gates and options for their solution are discussed.

Bibliography — 218 references.

Molecular modelling and calculations of the free energies of binding of proteins and biologically active compounds 211

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Computer-based numerical calculations of the structure and thermodynamics of microscopic models is an efficient tool for the study of molecular mechanisms of biochemical processes and reactivity of physiologically active compounds. The review considers statistical mechanical methods for calculation of free energies of equilibrium systems. The techniques enhancing the accuracy and efficiency of the free energy calculations are overviewed. Examples of calculation of binding thermodynamics for model protein-ligand complexes of bacteriophage T4 lysozyme and β -trypsin are given. The role and potential of molecular simulation methods in the modern drug design are discussed.

Bibliography — 237 references.

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The review deals with the use of chitosan and its derivatives as vectors for delivery of nucleic acids in gene therapy. Factors influencing the transfection efficiency of polyplexes of chitosan and its derivatives (molecular weight, the degree of deacetylation, pH, type of chemical modification, type of transfected cells) are discussed. Particular attention is paid to methods of chemical modification of chitosan (covalent hydrophilic and hydrophobic modification and non-covalent modification), which are able to increase the transfection efficiency and to provide targeted delivery of nucleic acids.

Bibliography — 151 references.

Indium iodides

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Indium iodides have been studied for more than 100 years, the focus of the studies drifting with time from inorganic compounds and halogen fluorescent lamp components to indium complexes and (in the current century) to organoindium compounds. The review surveys the properties of the iodides InI₃, InI₂ and InI, the phase diagrams of systems involving these iodides, structural data and complexes they form. Some discrepancies in the published data are noted. The existence of some compounds that are yet to be described is predicted. Indium monoiodide and its derivatives are of interest as radiation detector materials and for infrared photonics. The physical and chemical problems of application of indium iodides in halogen lamps are considered. A detailed review of patents on this topic is given. Chemical reactions of indium iodides used in organic synthesis and the types of organoindium compounds thus formed are discussed.

Bibliography — 316 references.