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Contents

Macrocyclic cavitands, cucurbit[*n*]urils: prospects for application in biochemistry, medicine, and nanotechnologies

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The prospects of using organic macrocyclic cavitands, cucurbit[*n*]urils (CB[*n*]) and their derivatives, in biochemistry, medicine and nanotechnologies are considered. The combination of CB[*n*] characteristics such as rigid highly symmetrical structure, polarized hydrophilic portals, rather large hydrophobic intramolecular cavity, as well as high stability to thermolysis and corrosive media and low toxicity account for the broad range of unique opportunities for the deliberate design of new functional materials, which could find application in various areas of modern chemistry and new technologies. The inclusion compounds of CB[*n*] with biologically active molecules demonstrate a high potential for the development of a new generation of prolonged action pharmaceuticals. The review presents the prospects for application of CB[*n*] for the manufacture of unique materials, CB[*n*]-containing vesicles, films and surfaces suitable for immobilization of various molecules and nanoparticles and for the separation of complex mixtures. The potential applications of CB[*n*]-modified electrodes and hydrogels and the use of CB[*n*] in proton-conductive materials and gas sorption and separation materials are discussed.

Bibliography — 164 references.

Methods for annelation of the furan ring to arenes

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Owing to their unique physicochemical, chemical and biological properties, benzo[*b*]furans have found application in various fields of chemistry and engineering. First of all, mention should be made of the broad range of biological activities of natural and synthetic derivatives of benzo[*b*]furan and its fused analogues (naphthofurans, anthrafurans and so on), which accounts for researchers' interest in the use of these heterocycles as important building blocks in drug design. The review considers the methods of furan ring annelation to arenes developed mainly in the last decade. The trends of development of methods for benzo[*b*]furan synthesis, some of which have been proved efficient for the preparation of polyfunctional compounds, are analyzed.

Bibliography — 110 references.

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Published data on fullerenes which obey the isolated pentagon rule from C₇₂ up to C₈₆ are generalized. Analysis of the unstable isolated-pentagon-rule fullerenes is carried out and the instability criteria are formulated. Two main reasons for the instability of isolated-pentagon-rule fullerene molecules are identified: their radical nature and/or high local strain. The classification of fullerenes is performed and a revised isolated pentagon rule is presented.

Bibliography — 119 references.

Computer-aided prediction of xenobiotic metabolism in the human body

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The review describes the major databases containing information about the metabolism of xenobiotics, including data on drug metabolism, metabolic enzymes, schemes of biotransformation and the structures of some substrates and metabolites. Computational approaches used to predict the interaction of xenobiotics with metabolic enzymes, prediction of metabolic sites in the molecule, generation of structures of potential metabolites for subsequent evaluation of their properties are considered. The advantages and limitations of various computational methods for metabolism prediction and the prospects for their applications to improve the safety and efficacy of new drugs are discussed.

Bibliography — 165 references.

New electrochemical sensors with electrodes based on multilayers synthesized by layer-by-layer chemical assembly and their analytical potential

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The results of studies dealing with the use of layer-by-layer chemical assembly for the fabrication of multilayers on the electrode surface in order to develop electrochemical sensors for quantification of concentrations of inorganic, organic and bioorganic compounds are integrated and analyzed. The essence of the method is outlined and its key advantages are noted, such as the possibility of synthesis of single layers with a specified thickness and composition under mild conditions and of preparing multilayers on the basis of these layers. Charge transfer conditions in the layers on the electrode surface between the analyte molecules and redox sites of the electrode and functioning conditions of the optimal electrode are considered. The role of electrocatalysts and intermediates of these processes is noted. Particular attention is devoted to the methods of synthesis of gold nanoparticles of different size. The experimental results are presented and the prospects of application of layer-by-layer chemical assembly for the fabrication of electrodes for various electrochemical sensors are discussed.

Bibliography — 241 references.