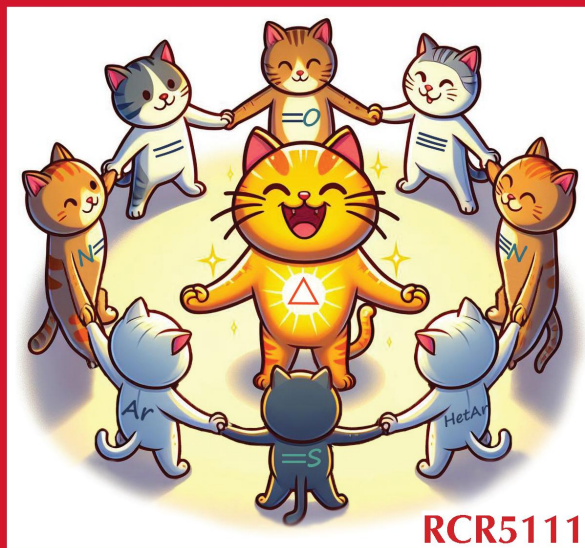


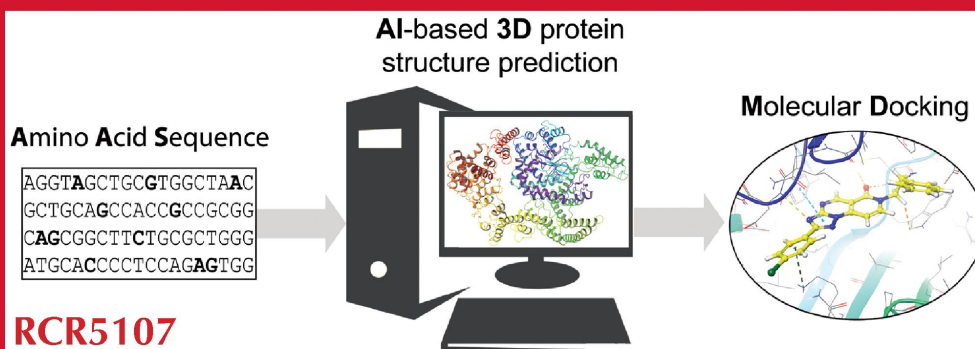
Natural additives with antimicrobial action used in dentistry

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|---|--|--|
| <p>Endodontics</p> <p><i>Thymus lamiaceae</i></p> <p><i>Origanum vulgare</i></p> <p><i>Colocasia esculenta</i></p> <p><i>Psidium guajava L.</i></p> <p><i>Amorphophallus paeoniifolius</i></p> <p><i>Epilobium parviflorum</i></p> | | <p>Therapeutic dentistry</p> <p><i>Lespedeza cuneata</i></p> <p><i>Lawsonia inermis</i></p> <p><i>Quercus infectoria</i></p> <p><i>Zanthoxylum achantopodium</i></p> <p><i>Scrophularia striata</i></p> <p><i>Sambucus williamsii</i></p> |
| <p>Orthodontics</p> <p><i>Cinnamomum verum</i></p> <p><i>Ulva lactuca</i></p> <p><i>Azadirachta indica</i></p> <p><i>Melaleuca alternifolia</i></p> <p><i>Padma hepaten</i></p> | | <p>Dental prosthetics</p> <p><i>Chamaecyparis obtusa</i></p> <p><i>Cinnamomum zeylanicum</i></p> <p><i>Turbinaria conoides</i></p> |

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AlphaFold for a medicinal chemist: tool or toy?

RCR5107

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The development of novel small drug molecules can be attributed to complex and important cross-disciplinary tasks. In the early stages of development, chemoinformatics and bioinformatics methods are routinely used to reduce the cost of finding a lead compound. Among the tools of medicinal chemistry, docking and molecular dynamics occupy a special place. These methods are used to predict the possible mechanism of binding of a potential ligand to a protein target. However, in order to perform a docking study, it is necessary to know the spatial structure of the protein under investigation. Although databases of crystallographic structures are available, the three-dimensional representations of many protein molecules have not been reported. There is therefore a need to model such three-dimensional conformations. Several computer algorithms have been published to solve this problem. AlphaFold is considered by the scientific community to be the most effective approach to predicting the three-dimensional structure of proteins. However, the scope of its application in medicinal chemistry, especially for virtual screening, remains unclear. This review describes methods for predicting the three-dimensional structure of a protein and provides representative examples of the use of AlphaFold for the design and rational selection of potential ligands. Special attention is given to publications presenting the results of experimental validation of the approach. Based on the analysis carried out, the main problems in the field and possible ways to solve them are formulated.

Bibliography — 154 references.

Progress in dental materials: application of natural ingredients

RCR5108

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The existing additives for dental restorative materials used in therapeutic dentistry, dentures, orthodontic appliances and adhesives (for example, metal and metal oxide nanoparticles) and also additives to root canal irrigants used in endodontics and to mouthwashes can be toxic to humans, cause allergic reactions and accumulate in organs and tissues. Today, a relevant trend is development of dental materials that have an antimicrobial effect and are non-toxic to humans. A promising alternative to the above-mentioned additives are phyto-components, including plant and propolis extracts, since they are cheap and non-toxic. This review is devoted to natural antimicrobial additives to dental materials used in orthodontics, dentures, therapeutic dentistry and endodontics. The review makes recommendations regarding additional research required for practical implementation of the considered dental materials (filling materials, mouthwashes, orthodontic adhesives and orthopaedic dental products), examines the influence of antimicrobial additives on the physicochemical and physicomachanical properties of polymer dental materials, and outlines the advantages and disadvantages of natural additives compared to synthetic ones. The main challenges in this research area are the narrow range of microorganisms for which the antimicrobial effect was studied (which are mainly *S. mutans*, *E. faecalis*, *C. albicans*) and the predominance of *in vitro* studies over clinical studies. The review covers published data of the past five years.

Bibliography — 123 references.

Cyclization reactions of cyclopropane derivatives with conjugated carbo- and heterosystems

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The strained structure of cyclopropanes serves as a kind of trigger for a variety of chemical transformations. Among others, processes involving conjugated unsaturated systems are of particular interest. The systems of unsaturated bonds are characterized by the possibility of flexibly varying their reactivity up to their full involvement in transformations. This review is the first to consider options for implementing the idea of combining the strain energy of cyclopropanes and the synthetic capacity of conjugated unsaturated systems within a single concept. A detailed analysis of processes involving activated cyclopropanes and numerous carbodiene and heterodiene systems is presented.

Bibliography — 289 references.