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Introduction to the Thematic Issue on Biologically Active Coordination Compounds

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The clinical implementation of new synthetic pharmaceutical drugs aimed at combating socially significant diseases is a part of national security of the country.

In recent decades, a segment of drug substances containing a metal atom in the molecule has formed in the pharmaceutical market. Metal complexes show a wide range of biological activities, including antitumor, antibacterial, anti-inflammatory, antiviral, and other types of activity. The use of metal-based drugs for diagnosis (metallodiagnosis) and therapy (metallotherapeutics) of socially significant diseases opens up unique opportunities for treating the pathologies that could not be treated by conventional organic drugs. The most well-known examples are platinum, gold, gallium, lithium, gadolinium, lanthanum, antimony, and bismuth compounds implemented in the clinical practice in the 20th century. Therefore, the search for new drug candidates among metal compounds appears to be an important and relevant task. This trend that appeared at the border between two intensively developing fields, medicinal chemistry and biological inorganic chemistry, has been called "inorganic medicinal chemistry."

In the modern medicinal chemistry, rational design of new physiologically active compounds is based on the key concept of a target, i.e., on the deliberate design of target-oriented molecules. The drugs designed in this way are called targeted drugs. Furthermore, the development of new metal-based pharmaceuticals opens up additional possibilities for the search for new targets and new mechanisms of action.

A strategic goal of the search for pharmacologically active metal complexes is to move away from the total screening and simple assumptions, but to strictly follow the medicinal chemistry concept based on the molecular design of compounds (in this case, metal-based compounds) in accordance with their ability to bind to the biological target that is involved in the pathogenesis of a particular disease. The major obstacle in this area is the difficulty of using *in silico* methods, i.e., molecular modeling, molecular dynamics, etc., and, generally, selecting the structures that bind to the target sites, due to the presence of a heavy metal atom.

As a result, several strategies for the assembly of metal-based active molecules are used. These strategies appeared historically and they can be classified into several basic methods:

(1) optimization of molecular structures of known metal-based drugs (the molecular action mechanism and/or the target are known);

(2) activation of an organic drug molecule by introducing a metal atom (the target for the organic drug is known);

(3) combination of a known organic drug and a metal atom with proven pharmacological activity to form a hybrid molecule (one or both targets are known).

Two thematic issues (9 and 10) of the *Russian Journal of Coordination Chemistry*, devoted to biologically active coordination compounds, include papers that describe various approaches to the synthesis and studies of the properties and biological activities of the coordination compounds of platinum, palladium, copper, cobalt, iron, zinc, gold, gadolinium, europium, neodymium, etc. The attention is focused on anticancer and antiviral activities, which is due to the modern challenges and the strategic need to develop new effective and safe pharmaceutical drugs.

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