STATE-OF-THE-ART APPROACHES TO CREATING METAL-BASED DRUGS

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DOI: 10.19163/MedChemRussia2021-2021-112

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The presentation will focus on novel approaches to constructing physiologically active metal-based drugs candidates based on target-oriented design, new synthetic approaches and extensive biological screenings. This study is focused on the design of hybrid compounds possessing 2,6-dialkylphenol group with dual modes of action – prooxidative and antioxidative activities. The presence of metal atom allows extensive modification including coordination to the targeted specific groups to control and tune toxicity-activity profiles. The synthesis and biological activity will be discussed. The anti/prooxidant activity has been studied in *in vitro*, *ex vivo*, *in vivo* experiments. We used general strategy of medicinal chemistry in the design of metal (Au, Sn) containing drug candidates, that is, rational selection of validated target, computer assisted molecular design, directed synthesis and screening.

The work has generated the libraries of organic ligands and organometallic and coordination compounds. Newly synthesized compounds were studied for their physico-chemical properties, reaction capability, interaction with cellular targets including molecular docking, and finally, potency *in vitro* and *in vivo*. As a result, several lead compounds mostly organotinins have been selected for further in-depth investigation.

This work was supported by RSF (19-13-00084).

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