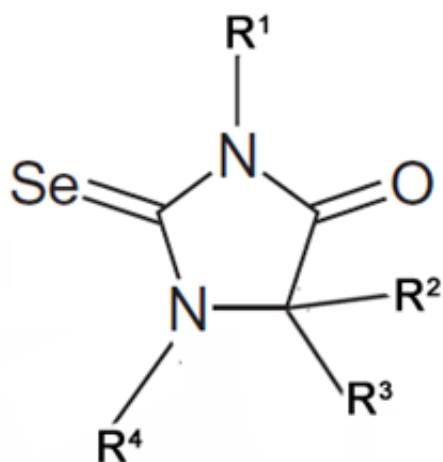


Scientists synthesize new molecules with anticancer and antioxidant activity

March 15 2016



General formula of selenohydantoins. Credit: Y. Ivanenkov et.al. *Bioorganic & Medical Chemistry* (2016)

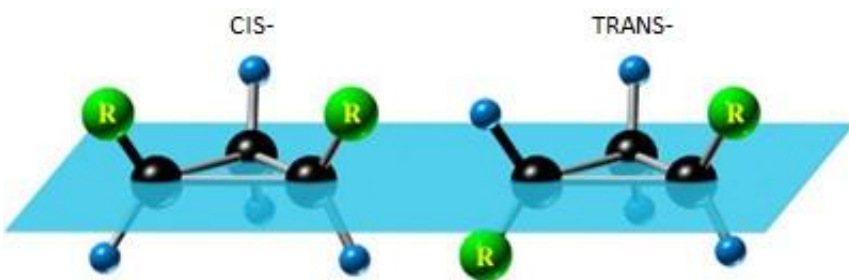
A group of scientists from Moscow universities led by Yan Ivanenkov, the head of Laboratory of Medical Chemistry and Bioinformatics in MIPT, has succeeded in synthesizing a set of novel selenohydantoins with anticancer and antioxidant activity. The corresponding paper has been published in the scientific journal *Bioorganic & Medicinal Chemistry*.

It was found that synthesized [molecules](#) could potentially be used as [anticancer](#) agents with good selectivity index. Hydantoin moiety and its derivatives can be found in many drug molecules, including nilutamide,

which is used in chemotherapy for prostate cancer, and dantrolene, which helps to relax skeletal muscles and prevent cramps.

Selenohydantoins are derivatives of hydantoins in which one of the oxygen atoms is replaced by selenium. It was found that drug molecules containing selenium possess anticancer activity and can be used as effective antioxidants. Selenium can be found in a number of known [drug molecules](#), such as Ebselen, an antioxidant with a broad spectrum of therapeutic activity.

In the study, the scientists have synthesized novel selenium-containing hydantoin derivatives. The structures of the molecules obtained were confirmed by NMR (Nuclear Magnetic Resonance) spectroscopy, high resolution mass spectrometry, and X-ray analysis. It was found that in the presence of Cu^{2+} copper cations, a spatial transformation is observed and a stable isomer is formed.



In the cis-configuration, the radicals (green) are on one side of the plane of the molecule, in the trans-configuration they are on opposite sides. Credit: orgchem.ru

Isomers are molecules with the same atomic composition, but different spatial structure. The interest lies in the fact that the isomers differ in terms of their properties and activity. The scientists used quantum-

chemical calculations to explain the mechanism of the transformation they had discovered.

The results of electromechanical studies showed that the synthesized molecules possess [antioxidant activity](#), which means they are able to slow down the process of oxidation. They are also able to bind to receptors that protect the body from oxidation.

"We have examined the effect of selenium on the activity of the synthesized molecules. The next step is to investigate the pharmacological potential of the most active molecules in vivo and in vitro," said Yan Ivanenkov, the head of the Laboratory of Medical Chemistry and Bioinformatics, when commenting on the prospects of the research.

The results of the study highlighted the important role of [selenium](#) in the structure of hydantoin derivatives. Structural modification such as this has a significant influence on the spectrum of biological activity and properties of the molecules.

More information: Yan A. Ivanenkov et al. Synthesis, isomerization and biological activity of novel 2-selenohydantoin derivatives, *Bioorganic & Medicinal Chemistry* (2016). [DOI: 10.1016/j.bmc.2015.12.050](#)

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