New method will make doping tests quicker
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Skoltech scientists and their colleagues proposed a way to simplify the search for traces of medicines, narcotic substances and sports doping drugs in human biological samples by performing two additional tests with the search domain reduced tenfold. Their research was published in the journal *Analytical Chemistry*.

Scientists determine the chemical composition of a substance using mass spectrometry: as neutral molecules and atoms turn into charged ions, the mass spectrum, i.e. the components’ relative masses in the mixture, is determined based on the ions’ trajectories in the electromagnetic field. Mass spectrometry helps detect anabolics, diuretics and even artificial testosterone.

The mass spectrum is only half the battle, though. Open-access databases of chemical compounds, such as PubChem, contain upwards of 120 million entries. As for mass spectrum databases, they are limited to half a million compounds only. PubChem may deliver several thousand compounds that match the molecular formula reconstructed using the mass spectrum.

Yury Kostyukevich, an associate professor at the Skoltech Center for Computational and Data-Intensive Science and Engineering (CDISE), and his colleagues put forward a method that helps reduce the search space, i.e. the multitude of options to choose from, by a factor of 10, which makes the formidable search task much easier by offering more information on the molecule structure.

The scientists suggested supplementing the standard mass spectrometry routines with two tests exploiting the exchange reactions that involve light and heavy hydrogen and oxygen isotopes (16O and 18O). The test results shed light on the molecule structure and serve as a filter in selecting suitable compounds.

The scientists tested their method on methylenedioxyxpyrovalerone (MDPV), a stimulant listed among controlled narcotic drugs, psychotropic substances and their precursors according to Russian law. MDPV is perfectly suitable for the purpose, since its formula, C16H21NO3, delivers 19,337 matches, of which only seven compounds have ready mass spectra. The two fairly simple tests proposed by the authors reduce the search domain by 13 times, limiting it to 1,515 molecules. According to Kostyukevich, only a small fraction of them are of biological origin, which makes things much easier.

The idea behind the new method will work even for previously unknown types of doping. “Our tests help detect a substance that other athletes do not have in their samples and see what the compound looks like. Then it will be up to sports physicians to figure out if the athlete took an illegal drug or had some exotic food the previous day,” Kostyukevish explained.


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