At the Faculty of Chemistry of Moscow State University. MV Lomonosov has developed an algorithm capable of finding the missing spatial forms of molecules, which is important for accurate modeling of new compounds. We are talking about the so-called conformations-various geometric versions of the same molecules arising due to the rotation of its individual parts.

Existing methods do not always reveal all possible options, which can lead to errors when creating drugs or other active substances. A new approach using artificial intelligence helps to compensate for these defects.

The algorithm first uses quantum-chemical calculations to study how the energy of the molecule changes when turning its parts. After that, the program analyzes the already built geometry and finds those that could be missed. Unlike traditional methods, the system is not limited to the search for only the most stable form, but explores a wider range of possible options.

When testing the method for 60 molecules for almost half of them, they managed to find up to 28 new forms that were not detected in other ways. This increases the accuracy of modeling and can accelerate the creation of organic and metal -organic compounds with the desired properties.