Product recommendation systems can help with search of antiviral drugs

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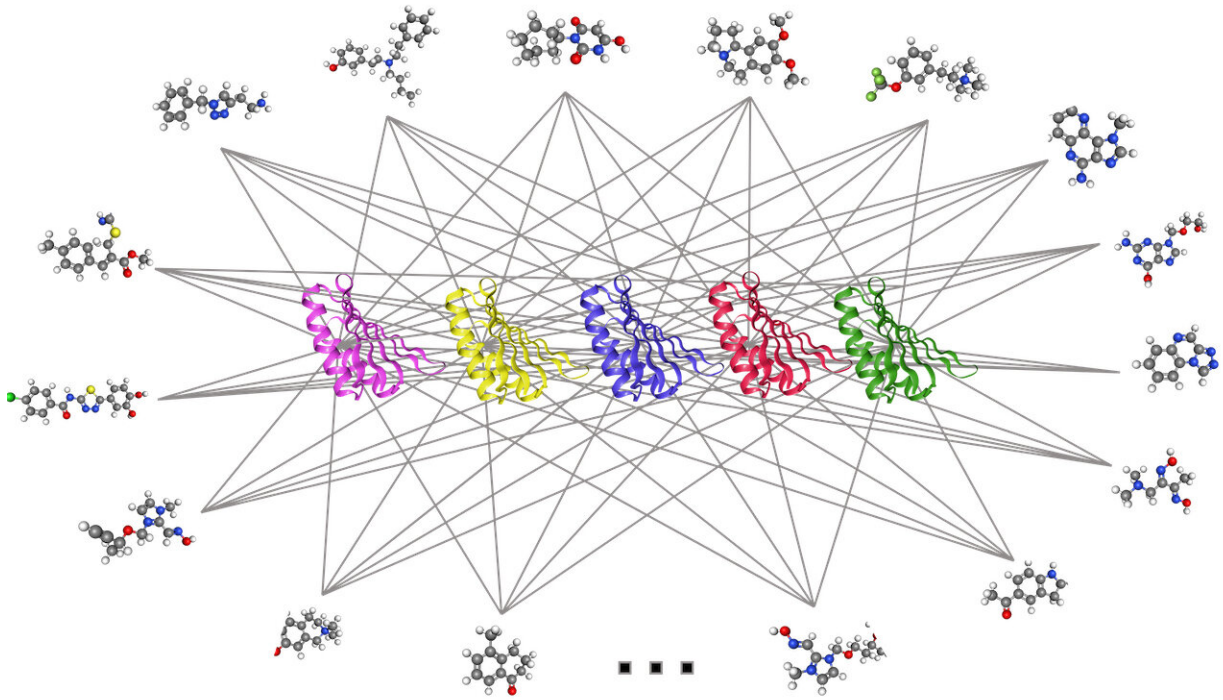

Active compounds search in broad chemical space. Credit: Skoltech

Scientists from Skoltech and the Chumakov Federal Scientific Center for Research and Development of Immune-and-Biological Products of RAS evaluated the ability of artificial intelligence that suggest products

to buy and recommend new antiviral compounds. The researchers found that advanced algorithms can effectively suggest both music, movies to buy, and compounds with antiviral activity.

Every internet user knows contextual advertising that suggests products to buy along with already purchased ones. Online retail use recommender systems that analyze user's preferences and purchase history to suggest a new product, a movie, or music. Can these algorithms 'recommend' a new antiviral drug or 'recommend' a well-known approved drug for a new disease?

A multidisciplinary team from the Skoltech Center for Computational and Data-Intensive Science and Engineering (CDISE) (Ekaterina Sosnina, Sergey Sosnin, Ivan Nazarov, and Maxim Fedorov) and the Chumakov Federal Scientific Center for Research and Development of Immune-and-Biological Products of RAS (Anastasia Nikitina and Dmitry Osolodkin) has investigated this idea. The researchers carried out computational experiments and compared the performance of different recommender algorithms for the selection of small molecules active toward viruses.

They showed that recommender systems could effectively pinpoint antiviral compounds and find promising drug candidates based on latent relationships in chemical and biological data. The key to success was Big Data: the team used the extensive ViralCHEMBL database containing antiviral activity data of about 250,000 molecules against 158 viral species.

"The success of this project is based on both significant progress in the mathematical algorithms and deep expertise in the subject area, such as medicinal chemistry, biology, and machine learning. We launched this project long before the coronavirus outbreak and hope that our findings will help researchers to find new molecules with anti-SARS-CoV-2

activity," says Ekaterina Sosnina, a Ph.D. student at Skoltech and the first author of the paper.

The scientists believe that their study will help chemists to find new antiviral drug candidates and provide a way for the repurposing of the existing drugs to combat SARS-CoV-2 and other potential viral outbreaks.

More information: Ekaterina A. Sosnina et al, Recommender Systems in Antiviral Drug Discovery, *ACS Omega* (2020). DOI: 10.1021/acsomega.0c00857

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