# Drug discovery platform may provide new options for treating mental health illnesses

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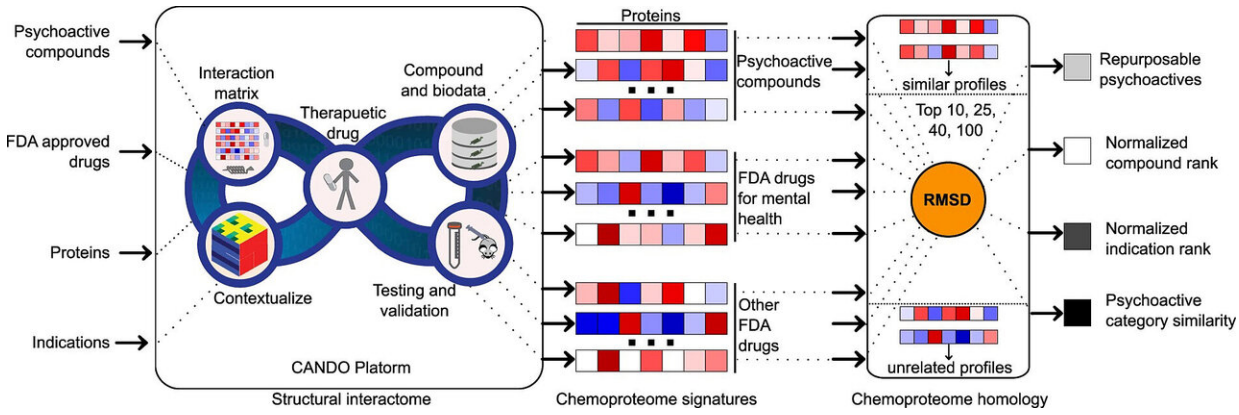


Schematic of computational chemoproteomics pipeline to identify psychoactives for mental-health indications using the CANDO platform. Credit: Purdue University

An estimated 46.6 million U.S. adults struggle with mental illnesses, such as anxiety disorder, according to the National Institute of Mental Health. About half of millennials and 75% of Gen-Zers report having quit jobs for mental health reasons.

Now, Purdue University scientists have created a platform focused on finding new medication options for people dealing with mental illnesses. The Computational Analysis of Novel Drug Opportunities (CANDO) drug discovery platform is designed to predict the effectiveness of

certain psychoactive drugs, which act primarily upon the central nervous system. Details about the platform are published in the Sept. 11 edition of *Scientific Reports*.

"One of the areas we are looking at with the platform is the use of non-addictive cannabis-based drugs that may help people with mental illness," said Gaurav Chopra, an assistant professor of analytical and physical chemistry in Purdue's College of Science, who led the creation of the platform. "Our approach is unique because we look at compound interactions with the entire proteome, rather than the traditional approach of focusing on the interaction with just one target or just by looking at the structure of the drug."

The CANDO drug discovery platform analyzes how a drug may work for a certain mental illnesses, based on a collective comparison with all other drugs already approved to treat those same conditions or symptoms of the underlying disease. The platform also looks for signature compound interactions with proteins that are similar in the proposed drugs with those already being used to treat people.

"Our goal with this platform is mapping potential uses for selected drugs to serve as a starting point to ignite further research into the once forbidden field of mental illnesses," Chopra said. "Our work on compound interactions of all known psychoactive substances provides a resource to further verify the use of selected psychoactives, identify mechanisms of action and suggest relationships between different mental health indications. This will enhance research in drug discovery for several mental health conditions as well as help with identifying mechanisms for eventual treatment of indications such as pain and substance use disorder."

**More information:** Jonathan Fine et al. Computational chemoproteomics to understand the role of selected psychoactives in

treating mental health indications, *Scientific Reports* (2019). DOI: 10.1038/s41598-019-49515-0

More information about the lab's work is available at github.com/chopralab/candiy_fun

Provided by Purdue University