

LBRN 19th Annual Meeting



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Broad spectrum coronavirus therapeutic discovery using the CANDO platform : We developed the Computational Analysis of Novel Drug Repurposing Opportunities (CANDO) platform for shotgun multitarget drug discovery, repurposing, and design, funded in part by a 2010 NIH Director's Pioneer Award, to rapidly deal with the

type of scenario caused by the COVID-19 pandemic. The multiscale platform screens and ranks every existing human use drug for every disease/indication through large scale modelling, context-sensitive design, and predictive bioanalytics of interactions between comprehensive libraries of drugs/compounds and protein structures. We utilised the CANDO platform to predict new uses of existing drugs for the rapid treatment and prophylaxis against SARS-CoV-2 and other coronaviruses. 10/50 top predictions by CANDO against SARS-CoV-2 have been validated by us, our industry partners or by other groups (see <https://www.sciencedirect.com/science/article/pii/S1359644620301938>). A number of other drugs are ranked better that have yet to be validated (full list available at <http://protinfo.compbio.buffalo.edu/cando/results/covid19/>). The talk will describe the latest version of the CANDO platform (v2 going to v3) and its application to identifying and designing broad spectrum coronavirus therapeutics. We will present the latest results obtained both in general performance and specifically against COVID-19, as well as the challenges that were encountered and the approaches devised to overcome them.

Keynote talk Saturday February 13th, 2021 - 8:30 am (Central Time)



Virtual Meeting
February 12-13, 2021