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COMPUTATIONAL INSIGHTS INTO THE ORIGIN OF SARS-COV-2

AND REPURPOSING OF DRUGS FOR COVID-19

Date

MAY 27, 9 AM CEST

by

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In the last 20 years the world has been threatened with three different coronavirus (CoV) pandemic threats from Severe Acute Respiratory Syndrome coronavirus (SARS CoV) starting in 2002, Middle East respiratory syndrome coronavirus (MERS-CoV) in 2012 and finally COVID-19 due to SARS-CoV-2 in late 2019. All these posed serious global pandemic threats with estimated case fatality rates of 15% for SARS, 34% for MERS and 1-3% for SARS-CoV-2 (1). With the current pandemic still far from over, there is an urgent need to understand where the virus came from, and to find new drugs to treat COVID-19, the disease caused by SARS-CoV-2. We can assume this will not be the last coronavirus to threaten humanity, hence we need better tools to track virus origin, and to identify drugs active against future coronavirus threats. **In this seminar I discuss in silico computer modelling and screening approaches to estimate the SARS-CoV-2 susceptibility of humans and other important animal species. I will also illustrate how state-of-the-art computational methods can rapidly identify drugs from existing drug libraries that might be able to be repurposed to treat COVID-19 patients.** We also describe how this computational screening pipeline can be expanded in the future to identify drugs with broad spectrum activity against a wide diversity of coronaviruses. Individual drug protection to CoVs may be short-lived, given their rapid mutation rates and the development of drug resistance. Thus, CoV drugs should hit multiple targets within viruses to minimize resistance. For example, one of the key and surprising findings of our drug screens to date is the anthelminthic drug Ivermectin is able to inhibit multiple SARS-CoV-2 protein targets, potentially making it difficult for SARS-CoV-2 to develop resistance to it. I will describe the current state of development of in silico CoV drug screening, the challenges and pitfalls of these approaches, and our predictions of how such methods may be used to develop drugs for future CoV pandemics even before they occur.).

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David Winkler has an unusually broad formal training in chemistry, physics, chemical engineering and radioastronomy. He is a Professor of Biochemistry & Genetics at La Trobe Institute for Molecular Science at La Trobe University, an adjunct Professor of Medicinal Chemistry at the Monash Institute for Pharmaceutical Sciences, a visiting Professor in Pharmacy at the University of Nottingham, and a Fellow in evolutionary robotics at CSIRO Data61. He previously spent over 30 years at CSIRO researching the application of computational chemistry, AI, and machine learning methods to the design of drugs, agrochemicals, nanomaterials and biomaterials.

He is ranked 227th out of 81,000 medicinal chemists, and 999th out of 520,000 chemists worldwide (Mendeley 2019). He has authored over 200 refereed journal articles and book chapters, has an H index of 50, and is an inventor on 25 patents. He has won several prestigious awards including the CSIRO Medal for Business Excellence, RACI's Adrien Albert award for contributions to medicinal chemistry, the ACS Herman Skolnik award for excellence in cheminformatics, and a Royal Academy of Engineering (UK) Distinguished Fellowship (bioengineering). He is past President of the Federation of Asian Chemical Societies (FACS) and the Asian Federation for Medicinal Chemistry.

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