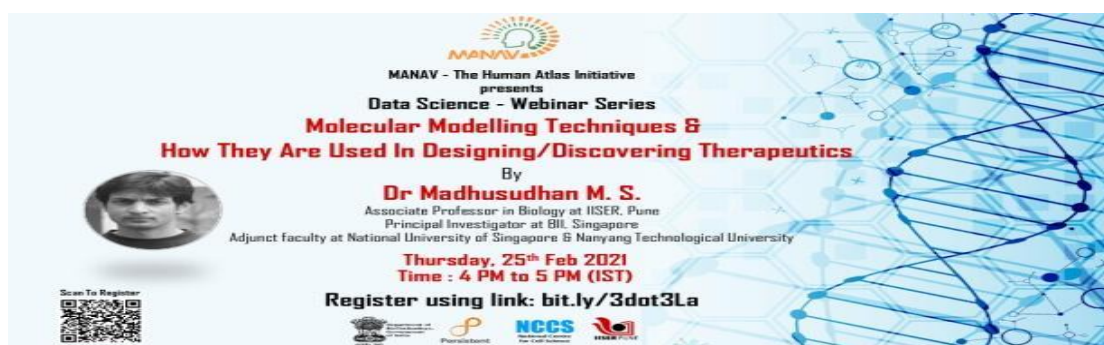


Webinar on how computational modelling aids drug discovery

New Delhi, March 10: Drug discovery is no longer restricted to experiments in a wet laboratory, even though such investigations in the laboratory play an important role. For example, they help determine the 3D structures of proteins, which is usually a key step in determining its functional role in the cell. These structures are often determined when the molecule is interacting with other molecules, which provides hints to how the protein molecule might function inside the cell. However, the determination of such structures experimentally is not always easy or possible. When this is the case, other methods like computational modelling and prediction tools can be used to accomplish the same goals. Such tools are useful to discover or design therapeutic agents against particular targets.



MANAV - The Human Atlas Initiative
presents
Data Science - Webinar Series
**Molecular Modelling Techniques &
How They Are Used In Designing/Discovering Therapeutics**
By
Dr. Madhusudhan M. S.
Associate Professor in Biology at IISER, Pune
Principal Investigator at BII, Singapore
Adjunct faculty at National University of Singapore & Nanyang Technological University
Thursday, 25th Feb 2021
Time : 4 PM to 5 PM (IST)
Register using link: bit.ly/3dot3La

To create awareness about how computational modelling can aid drug discovery, a webinar on ‘Molecular modelling techniques and how they are used in designing/discovering therapeutics’ was organized by the ‘Manav: Human Atlas Initiative’ on Thursday, 25 February 2021. This webinar was presented by Dr. M. S. Madhusudhan. Dr. Madhusudhan is Associate Professor in Biology at IISER-Pune, Principal Investigator at BII, Singapore, and Adjunct Faculty at the National University of Singapore & Nanyang Technological University. Using the Nipah virus as a case study, he gave an overview of the different modelling techniques used, and how they can help look for potential drugs and vaccines.

This webinar is part of the data science webinar series organized under the auspices of the “Manav: Human Atlas Initiative”. This initiative is a collaborative project between the National Centre for Cell Science (DBT-NCCS), the Indian Institute of Science Education and Research (IISER-Pune) and Persistent Systems, and is funded by the Department of Biotechnology (DBT), Government of India, and co-funded by Persistent Systems. This series was initiated soon after the lockdown began, turning this challenging situation into an opportunity to create awareness about data science and its applications. These webinars are open to all, and have attracted thousands of registrations, mainly from students. The “Manav: Human Atlas Initiative” aims to annotate the extensive information related to the human body that is available in the scientific literature and databases, and initiate steps towards creating a human atlas eventually. The project, being conducted through a public-private

partnership, serves as a platform to help students across India learn how to comprehend and analyze scientific literature, and extract relevant information from it using a digital annotation tool. Online workshops on how to read scientific literature are also routinely conducted. Colleges interested in having a session organized for their students can write to manav.iiserpune@gmail.com. Students, faculty members and researchers interested in participating in the project can learn more from the project's website (<https://manav.gov.in/>) and social media: Twitter (Manav Human Atlas; @ManavAtlas) & Facebook (MANAV Human Atlas). The Rajya Sabha TV has also featured this initiative on Gyan Vigyan & Science Monitor.

Links related to this story -

*Twitter: @DBT_NCCS_Pune

https://twitter.com/DBT_NCCS_Pune/status/1362655940080660482

*Facebook: DBT - National Centre for Cell Science

https://www.facebook.com/509782325747597/photos/a.645426328849862/3860075960718200?notif_id=1613718654953192¬if_t=page_post_reaction&ref=notif

* YouTube Channel (archived webinars): Manav - The Human Atlas Initiative

* 'Manav: Human Atlas Initiative' featured by Rajya Sabha TV on -

Gyan Vigyan: <https://youtu.be/Ule08azR1ww>

Science Monitor: <https://www.youtube.com/watch?v=IMgTw6rXTGQ>

Contact Person & Contact Details communication coordinator: Jyoti Rao (jyoti@nccs.res.in)

Link: <https://www.nccs.res.in/>