Call for Papers: Special Issue on Computational Genomics and Molecular Medicine For Emerging COVID-19

TCBB seeks submissions for an upcoming special issue.

By controlling devastating and emerging coronavirus disease (COVID)-19, new drug molecules, vaccines and antibiotics from microbiological to sequence-based approaches have had an enormous impact on world health. Healthcare researchers have always been a leader in innovation. Virus diseases make it challenging to stay forward of the curve, but with the application and utility of artificial intelligence and machine learning algorithms, it continues to advance, creating new therapeutics will improve healthier lives. Intelligent algorithms for machine learning, as well as “big data,” are seen as calculation and support for COVID-19, but never as an objective in and of themselves. The improvements and recent growth that the use of pharmacogenomics and drug designing has seen in the past few years can cover fields that are directly or indirectly, or even be implemented to aid in the development of pharmaceutical products or industrial applications. As such, it is time to create a “Research Topic” where advances in this field, linked directly to COVID-19, are presented.

Currently, the People Republic of China and the number of Western countries are challenged with a huge burden of coronavirus infection to emerging COVID-19. The fact that a COVID-19 has emerged indicates immune naivety in the infected population, or altered virulence potential or an increase in the pathogen population. The rapid development of vaccines and therapeutics that target these pathogens is therefore essential to limit their spread. Genome sequences provide a previously unattainable route to investigate the mechanisms that underpin pathogenesis. Besides, genomics, transcriptomics, structural genomics, proteomics, and immunomics are being exploited to perfect the identification of targets, to design new vaccines and drugs, and to predict their effects in patients. Furthermore, human genomics and related studies are providing insights into aspects of host biology that are important in infectious disease.

Now, with the advent of the “machine learning on omics era,” a paradigm shift is occurring in the development of novel drug molecules, vaccines, and potential antibiotics are given that new motivation to this field. High-quality research related to drug design with genome engineering through artificial intelligence is an emerging field of study. It concerned with the design and testing of molecular properties, behavior and

interactions to assemble better materials, systems, and processes of COVID-19. Computational Artificial Intelligence and Chemistry advance is parallel with the rapid progress in drug designing methods. This technique is becoming a powerful tool in COVID-19 to identify the starting points as hit molecules. It reduces the time and cost-effective taken to drug development. Advances in artificial intelligence and small molecule chemistry are becoming the benchmark of the 21st century, opening up new avenues for drug discovery. New approaches are needed as the cost of COVID-19 drug development is increasing with decreasing investment returns. This ever-growing body of genomic data and machine learning-based approaches will play a critical role in the future to enable the timely development of vaccines and therapeutics to control emerging COVID-19.

Many challenges remain identification targets and in the processes needed to bring a new vaccine or drug to the market. Understanding the molecular nature of genomic segments/epitopes, the mechanisms of action of targets and drugs, and cell-mediated immunity are key priorities to be tackled in the coming years. These issues can be addressed by improved structural genomic studies of antigens and the compilation of databases containing information on structure, immunogenicity, and B and T cell epitope predictions through the advancement of machine learning. Numerous FDA-approved drugs are declining with the number of new molecular entities (NMEs). The reasons noted are adverse side effects and reduced efficiency of many potential compounds. Genome-based development of effective small molecule therapeutics and vaccines is still largely dependent on the availability of valid computational models to measure efficacy and protection against COVID-19. Artificial Intelligence and small molecule chemistry provide a new direction to the system-centric idea for R&D leading to future drugs, which starts with the identification of the scope of a new drug.

This special issue welcomes research that yields novel breakthroughs towards Artificial Intelligence and genome-based precision medicines for COVID-19. All the manuscripts submitted to this special issue will be peer-reviewed and accepted will be published in the *Special issue*.

Pertinent topics may include:

- Artificial intelligence in drug discovery and target identification for COVID-19
- Data mining and network analysis in COVID-19
- Structure, function, evolution and mapping of COVID-19
- Microarrays and next-generation sequencing in COVID-19
- Single cell transcriptomics of COVID-19
- Structural and target information for COVID-19
- Drug design and dynamics simulation for COVID-19
- Epitopes identification and vaccine design for COVID-19
- Human genomics and COVID-19

IMPORTANT DATES

Open for Abstract submission	: February 20, 2020
Open for submissions in ScholarOne Manuscripts	: March 15, 2020
Closed for submissions	: June 30, 2020
Results of first round of reviews	: August 15, 2020
Submission of revised manuscripts	: October 15, 2020
Results of second round of reviews	: November 15, 2020
Publication materials due	: December 01, 2020

SUBMISSION GUIDELINES

Prospective authors are invited to submit their manuscripts electronically after the “open for submissions” date, adhering to the *IEEE/ACM Transactions in Computational Biology and Bioinformatics* guidelines. Please submit your papers through the online system (https://mc.manuscriptcentral.com/tcbb-cs) and be sure to select the special issue or special section name. Manuscripts should not be published or currently submitted for publication elsewhere. Please submit only full papers intended for review, not abstracts, to the ScholarOne portal. If requested, abstracts should be sent by email to the guest editors directly.

GUEST EDITORS

Dongqing Wei, *Ph.D.,* is a professor of bioinformatics at Shanghai Jiaotong University since 2006. Over the past three decades he has made many grand breaking contributions to the development of molecular simulation techniques and their interdisciplinary applications to systems of ever-increasing complexity. He is best known for contributions to the development of molecular simulation, more recently, AI tools and software with applications to a wide range of chemical, physical and biological systems, from electrolytes, to polar liquids, to ferroelectric liquid crystals, to combined Quantum Mechanical/Molecular Mechanical (QM/MM) systems, to membrane proteins and protein-ligand complexes applied to computer aided drug design. His most important contributions in sciences are exemplified by the discovery of ferroelectric nematic liquids crystals, the first complete ab initio MD simulation of explosion (nitromethane), and anti-aging and anti-AD drug candidate WGX-50. Prof. Wei published more than 300 papers with citations of 8000 times.

Email:dqwei@sjtu.edu.cn

Aman Chandra Kaushik, *Ph.D.,* is an Assistant Professor at Wuxi School of Medicine, Jiangnan University, China. His research direction focuses on drug development for alzhimer, cancer and diabetes using machine learning and system biology approaches. He developed different machine learning tools Weidock, SPVec and A-CaMP have had an impact in system based medicine. Before Jiangnan University, he was a postdoctoral scholar in bioinformatics at Shanghai Jiao Tong University. He received his Ph.D. in Bioinformatics from the Gautam Buddha University, India while also researching at Ben-Gurion University of the Negev, Israel. He published more than 50 papers with citations of 200 times.

Email:amanbioinfo@sjtu.edu.cn

Gurudeeban Selvaraj, *Ph.D.,* is a MITACS-visiting Postdoctoral Scientist in Concordia University, Canada. He continues his research faculty position in Prof. Wei's lab, Henan Universtiy of Technology, China. His research investigates genomic and proteomic data to develop precision medicine for NSCLC using machine learning algorithms. He also involving vaccine design, statitcal meta-analysis of genomic and clinical data. Prior to joining CERMM, he has completed his postdoctoral reaserach in Henan Universtiy of Technology, and Istanbul Medeniyet University. He received his bachelor of science in Biochemistry from Bharathiar University, and his masters and doctorate in Marine Biotechnology from Annamalai University. He received research grant from different funding agencies includes MITACS Global link, China Postdoctoral Science Foundation, Henan Postdoctoral Science Foundation, Henan University of Technology, The Scientific and Technological Research Council of Turkey, and University Grants Commission, India. He published more than 50 research articles with scholary 1295 citations and H-index-19 in reputed journals including Current Medicinal Chemistry, Journal of Biomedical Informatics, Phytomedicine, The Journal of Physical Chemistry C and Current Pharmaceutical Design, Current Drug Targets and participated more than 25 different International and National conferences and workshops.

Email:gurudeeb99@haut.edu.cn

Yi Pan, PhD, is currently a Regents' Professor and Chair of Computer Science at Georgia State University, USA. He has served as an Associate Dean and Chair of Biology Department during 2013-2017 and Chair of Computer Science during 2006-2013. Dr. Pan joined Georgia State University in 2000, was promoted to full professor in 2004, named a Distinguished University Professor in 2013 and designated a Regents' Professor (the highest recognition given to a faculty member by the University System of Georgia) in 2015.

Dr. Pan received his B.Eng. and M.Eng. degrees in computer engineering from Tsinghua University, China, in 1982 and 1984, respectively, and his Ph.D. degree in computer science from the University of Pittsburgh, USA, in 1991. His profile has been featured as a distinguished alumnus in both Tsinghua Alumni Newsletter and University of Pittsburgh CS Alumni Newsletter. Dr. Pan's current research interests include parallel and cloud computing, big data, and bioinformatics. Dr. Pan has published more than

450 papers including over 250 SCI journal papers and 100 IEEE/ACM Transactions/journal papers. In addition, he has edited/authored 43 books. His work has been cited more than 12,200 times based on Google Scholar and his current h-index is 56. Dr. Pan has served as an editor-in-chief or editorial board member for 20 journals including 7 IEEE Transactions. Currently, he is Associate Editor-in-Chief of IEEE Transactions on Computational Biology and Bioinformatics. He is the recipient of many awards including one IEEE Transactions Best Paper Award, five IEEE and other international conference or journal Best Paper Awards, 4 IBM Faculty Awards, 2 JSPS Senior Invitation Fellowships, IEEE BIBE Outstanding Achievement Award, IEEE Outstanding Leadership Award, NSF Research Opportunity Award, and AFOSR Summer Faculty Research Fellowship. He has organized numerous international conferences and delivered keynote speeches at over 60 international conferences around the world.

Email: yipan@gsu.edu