INTERNATIONAL SOCIETY FOR
COMPUTATIONAL BIOLOGY

SUMMER 2021 | ISSUE 02

ISCBNEWSLETTER

CONTENTS:

COSI SCHEDULES

GET TO KNOW YOUR ISCB PRESIDENT:
CHRISTINE ORENGO

ISCB made history in January 2021 when it welcomed its first female president into office. Christine Orengo from University College London in United Kingdom succeeded Thomas Lengauer as ISCB's 8th president.

1. *Can you tell us a little about yourself and your background?*

I started my scientific life as a theoretical quantum chemist and my first paper was on vibrational levels in methanol – so its been an interesting journey! I was tempted by biology and amazed by the molecular machinery in cells so switched to molecular biology. My PhD was in mathematical modelling of redox enzymes. After a brief spell in industry improving my computational skills, I worked at the National Institute of Medical Research in London on algorithms to compare protein structures and detect evolutionary relationships. I was enormously fortunate to be supervised by two brilliant scientists, Willie Taylor and then my luck took me to the lab of Janet Thornton, who had the great idea to set up an evolutionary classification of proteins. The CATH classification was established in 1994 and data from that is still at the heart of many of the algorithms and analyses conducted by my group. In 1995, a ten-year fellowship gave me freedom to pursue new interests in functional genomics (e.g. to analyse protein networks and disease associations). Subsequently, becoming a professor at UCL gave the security and then funding to explore other avenues and establish research collaborations with experimental groups. I've been fortunate to have very talented, collaborative researchers in my team and we've participated in many exciting European (e.g. BioSapiens, Integr8, EMBRACE, ENFIN, IMPACT, IMI-PAIN) and American (MCSG, CSGID) consortia. Ian Sillitoe, in my team, has driven development of CATH and ensured it remains robust and representative, reflected in recent endorsement as a Core Data Resource by the European ELIXIR initiative. Our algorithms for protein function prediction were respectably ranked in the CAFA assessments, and we are now having a lot of fun exploring new machine learning strategies for them.

My election to the Royal Society in 2019 was also a testimony to the dedication and innovation of my team. I've been fortunate to spend my working life doing what I love with scientists, both inside my team and out, who are truly generous and collaborative.

I've been involved in ISCB since 2011, first on the Board of Directors and then a Vice President in 2014. I helped establish the COSIs – Communities of Special Interest, in order to better highlight their cutting-edge research and improve networking. I've also been Co-Chair of Conferences and on the Awards and Fellows Committees. Outside ISCB I'm co-leading the European ELIXIR 3D-BioInfo Structural Bioinformatics Community and co-lead the Genomics England Functional Effects Domain. I've served on Royal Society Committees and was appointed last year to the Council of the UK's largest funder of biological and biotechnological research (BBSRC). Finally, I'm also a trustee of a small charity working in Madagascar on education and environmental projects.

2. How has the field of computational biology and bioinformatics changed from when you entered to the field to now?

It has changed enormously and I think we're on the cusp of a defining era in biology with the explosion of data over the last twenty years and new technologies for data science. When CATH was launched 25 years ago, it only had ~3000 experimentally determined protein domain structures in it – now it has more than half a million! The predicted structural data has increased more than 300 fold! Furthermore, new data types emerged, that allowed systems based approaches to understand how networks of proteins behave. Recent revolutions in single cell technologies will significantly increase the power of that data, bringing clearer insights on changes in the cell under different conditions.

The increasing proteomics data gives sharper focus on which processes proteins really engage in and metabolomics data insights on the chemistry linked to these processes. Alongside the data revolution, there have been radical developments in computational methodologies. For example, continuous improvements in text mining harness more of the vast wealth of information in the literature. Novel methods for linking data (eg knowledge-graphs) are enabling integration of very heterogenous data, revealing new associations. The expansion in the data also enabled more powerful AI strategies e.g. deep learning techniques. These are particularly exciting and have the potential to be hugely transformative for our field. The recent success of DeepMind's AlphaFold strategy in predicting protein structures (of comparable quality to experimentally determined structures) will revolutionise our understanding of protein mechanisms. These strategies can be applied to many other data types.

In addition to changes in the data and data science there have been significant cultural shifts. The diversity of data available means that some of the most exciting work involves multi-disciplinary teams where people have to learn each other's language and novel insights come from emergence of new perceptions and new ways of working. As a society we should work with scientific publishers to lobby for equal representation of our members in the accreditation for these collaborations and we need to find ways to further facilitate these cultural shifts.

3. How has the COVID 19 Pandemic impacted your work and in turn your view and vision for ISCB?

Covid-19 has surely impacted everyone's work! Its challenging to meet your team and collaborators only via zoom. These restrictions have been much easier for our community than for experimental scientists, though. Nevertheless good collaborations and team spirit need in-vivo nurturing. A silver lining is that we can have more meetings with collaborators as without travel it's easier to find times. We've reduced our carbon footprint too! That increased contact can really advance the research and give better integration of multi-disciplinary teams. Furthermore, despite the challenges, its astounded me how much can be done by zoom. My team have been more productive than ever! However, I fear work-life balance has suffered and we need to be careful about that.

One thing that has really impressed me is the willingness of people to share data and work collaboratively. We did a short study on SARS-CoV-2 which involved groups working with us via zoom from Malaysia, India and multiple institutes across the UK! And there have been many examples in the literature of very large consortia of researchers who have come together to rapidly find answers to the impact of variants, host genes implicated, the effect of drugs etc. In many countries, funding has been rapidly diverted to support these initiatives which I find reassuring as it shows agility and a desire and mechanisms to solve global issues quickly. We will likely need that again for future pandemics and climate issues.

ISCB is keen to benefit from these silver linings, particularly the ease with which researchers can collaborate and network by zoom and especially across continents. The virtual ISMB conference had nearly 2400 participants last year and we have over 2000 this year - many more people than would normally attend. Researchers from 75 countries have registered, this is a 25% increase in participation over ISMB 2019 when we were in person. We are really keen to increase membership and participation from researchers in Africa, Latin America and Asia and hybrid meetings offer those opportunities. Hybrid meetings could also be a good way of keeping our Communities of Special Interest (COSIs) active by supporting regional meetings throughout the year. People still seem keen to watch zoom webinars and the ISCBacademy is really picking up. We want to build on that and are planning a series of webinars, linked to the COSIs, highlighting exciting developments and introducing young rising stars. We are also hoping to have webinars around social issues. For example, the impact that research and discoveries in our field could have on society (AI and personalized medicine come to mind) and how we build a dialogue with the public around those and other ethical themes.

4. How has ISCB helped to grow or influence the field?

ISCB is an organic community of volunteers which I believe has played a significant role in helping computational biologists to learn about cutting edge research in their field. It's particularly important for young scientists, helping them to network and learn about new themes and opportunities. In fact in this year's ISMB 54% of participants are PhD students and postdoctoral fellows. Over the years, we have increased our global reach - the decisions to hold ISCB-X meetings in Africa, Asia and Latin America, introduced by Burkhard Rost, provided opportunities for scientists on these continents to meet more easily and network. Our Regional Committee also helps our scientists stay networked outside ISMB, through meetings closer to home.

Restructuring the society to support COSIs has helped in giving researchers in particular areas more focused opportunities to share research and discuss ideas. Indeed, the COSIs are shaping the research themes within ISCB, bringing leading players to their ISMB tracks for keynotes and often providing social events to enhance networking. Some COSIs have special mechanisms for highlighting key publications in their fields. Others are hosting assessments of major developments in the field (e.g. CAMDA, critical assessment of massive data analysis and CAFA, critical assessment of functional annotation).

ISCB has also supported the establishment of key forums for disseminating the community's research. The society contributed to the launch of PLoS Computational Biology and also Bioinformatics with top research selected for Proceedings Talks at ISMB routinely published in that journal. In the future, Bioinformatics Advances will also publish discoveries and developments in our field and we expect it to become a major forum for highlighting cutting edge research.

ISCB aims to be a beacon for fairness and diversity. We have established an Equity and Diversity Committee and will tread this path thoughtfully in a spirit of tolerance and understanding in order to bring everyone with us. We should be an exemplar for other societies and institutes. We have begun by surveying the balance in our committees and in the honours that we award. There is still some way to go, especially as regards nominations, but we have a very dedicated committee designing mechanisms that will enhance and support equality. On a positive note, the composition of our board and governance structures reflect well the gender ratio in ISCB, but more work needs to be done in other areas of diversity. ISCB aims to empower, award and connect researchers of every gender from every background, and every corner of the globe.

We have an energetic Education Committee, who are helping to shape curricula in our field, and enable ISCB affiliated courses. They participate in the Global Bioinformatics Education Summit and other important initiatives. Through the Public Affairs and Policy Committee, ISCB has also had an important advocacy role, lobbying to increase funding for our research and submit comments on national policies in support of our community. Through Green ISCB, we are also starting to examine the role we can play in advising on the carbon footprint our research activities impose and how we can provide information to help modify these impacts.

5. What are your goals for the society?

Ultimately, ISCB is what we as a community make it. The opportunity is there to do many new things. We are a very open and organic society. We have a fantastic operational team led by the highly professional and dedicated, Diane Kovats, but ISCB is also built on the good will of many volunteers. Crucially, we have a dynamic Board of Directors and Executive Committee - all are volunteers - with many ambitions and ideas for the society. As well as bringing my own ideas, my aim is to help them execute theirs, and persuade others to join us with new perspectives, making the society even more vibrant and representative.

I'd like to see ISCB building on its track record of promoting the latest, most exciting research perhaps by expanding the mechanisms for bringing scientists together. As regards training and enabling, we already have good programs and committed committees and task forces in these areas and we work with major global initiatives like Goblet and ELIXIR TESS, but given the wave of interest in new data science technologies and handling 'big data' we need to consider how to work more closely with neighbouring societies in computer science and engineering. Going back to the COVID silver linings, how can we help disseminate information about the vast amounts of on-line teaching material produced during the pandemic. Many institutes are switching to blended learning and might be eager to share their material and benefit from other institutes repositories. Can we help facilitate that?

Data sharing/stewardship and core bioinformatics have always been crucial for our field and we should be engaging with and supporting initiatives that support FAIR processes.

We have important aims around equality and fairness – increasing the representation of minority groups and ensuring everyone has a fair chance to present and participate in our meetings. I've already mentioned the Equity and Diversity Committee, but how can we persuade other members to get involved too. For example, the nominations we receive for ISCB Awards and Fellows are not diverse enough and we need ISCB members to be more proactive in nominations, in order to achieve a broader, fairer representation of our community.

We'd like to see our COSI communities expand and diversify their actions, becoming more active throughout the year. COSIs are run by committed and generous people who give a lot of their time to organize their annual programme tracks at ISMB. How can we help them to do more. Perhaps by tapping into our energetic student council and other young scientists with time and imagination to run COSI webinars or regional events. Let us know if you want to get involved or have other ideas for disseminating developments in your field and bringing researchers together. The ISCBacademy which advertises and hosts the webinars is becoming increasingly popular and we'd like talks in ISCB webinars to become a sought after distinction and on the checklists for career progression. Similarly, we want to increase the status of the Fellows – by making the process more transparent and bringing more diversity. A task force has already started working on that.

A recent major success, is the launch of the new ISCB Bioinformatics Advances journal. Started by Alfonso Valencia and the Publications Committee, this was supported and brought to fruition by Thomas Lengauer during his presidency. Bioinformatics Advances will both promote the science of our community and increase the profile of ISCB. We encourage members to submit their best work to this journal to ensure its success.

Finally, it will be important to engage with the public more since our technologies and discoveries contribute to advances in society but may also bring moral dilemmas e.g. around robotics and genetic engineering. Our Public Affairs and Policy Committee has just launched a 'Science in Society' series of webinars. The first will be at ISMB this year around the topic of Science Journalism and Science Communication. We welcome ideas for future conversations and volunteers willing to help with these 'Science in Society' webinars.

6. What do you believe are the biggest challenges to those goals facing ISCB?

In a post-Covid world money will be tight and ISCB must lobby wherever possible to protect the funding that is vital for our research. We must also identify inevitable impacts on ISCB e.g. financial shortfalls in conference and membership revenue, and build resilience into our plans for the future. The annual ISMB conference is our showcase event which lies at the heart of our role as community builder and which also brings the resources to support conferences in other countries, which need our support. Conference funding also helps support the ISCB professional team who work tirelessly to organize our conferences, our communities, our newsletters, our programs, our funding applications and all the other initiatives that support ISCB. Running ISMB 2020 and 2021 as virtual meetings has impacted our finances and we need to consider other mechanisms for enriching the society financially. Hopefully, our new journal, Bioinformatics Advances will help rescue us from the cliff edge, but other ideas need to be considered too. Again, we hope people will send ideas and join us to help where they have appropriate expertise.

As mentioned already, I believe another challenge is working out how to explain the radical new developments in our field to the people funding us and the people paying the taxes that support that funding. We need to spend more time communicating our science to the public!

7. What is your opinion of the programs offered by ISCB?

ISMB is one of the top Comp Bio meetings for hearing the latest advances, catching up with people in your field and exploring new themes and communities. The opportunity to be selected for Proceedings Talks, with publication in Bioinformatics, has promoted cutting edge science. The networking opportunities help many young researchers find new scientific ‘friends’ they can collaborate or communicate with throughout their careers.

Our new journal, Bioinformatics Advances is a really exciting development and has a very accomplished and diverse team of editors. The journal will report major developments and we aim for the journal to be read widely by our computational communities and even more widely e.g. experimental communities. It is a timely new forum as we move into a more multidisciplinary age.

Computational Biology is a very broad church now. ISCB captures diverse scientific interests through the COSIs. There are more than 20 of these now. What have we missed? We have programs to encourage COSIs to work together where interests overlap and we hope this will trigger new synergies. For many of the research themes, COSI meetings at ISMB have become major calendar events. ISMB special sessions publicise hot new topics – like the COVID-19 sessions Thomas Lengauer recently introduced. Can these sessions help shape new COSIs or expand existing ones?

The ISCB-X conferences established around the world (in Africa, Latin America, Asia) are flagships for our international aims. We are opening these up by supporting hybrid platforms for all our meetings to promote better interactions across our global community. We’re also looking into how we can broaden our advocacy programs.

Our honours – ISCB Awards and Fellowships are respected and sought after and certainly add weight to any CV. We will continue to increase their distinction by ensuring fair representation and transparent processes aligned with other highly respected societies.

We have a great education committee who have set up valuable programs for accrediting courses and bringing together trainers from across the world. This is needed more than ever. Data science is projected to occupy more than 80% of wet biologists time and they will increasingly seek help from us and join our ranks. It’s a great opportunity for ISCB to expand. Finally, our jobs boards help our members find new opportunities by publicising their CVs and availability.

8. What do you believe is the key to the success of ISCB?

Community and collaboration – we can achieve much more by helping each other and working together. Communication and transparency is also key, together with honesty. We need to explain what we do and what we want to change and be brave enough to take risks but also to own up to failures. We need to listen and understand what our members want and find ways to fund those changes. Inclusivity – we need to make sure that everyone is invited and has a place, and also has the means to take part. The benefits of hybrid meetings are the opportunity to share our science much more easily with scientists in every other corner of the world. We need to think about how to change the structure of our meetings and our society even more to enhance this. Talent – we need to attract the brightest and best to our committees to drive new ideas and change. Pride and humility – we need to talk more about our successes and accept our role in society, consider how our discoveries can help save the world or change it in radical ways that could be scary to some people. We need to explain our science better and win support from the public who fund us.

Over to you now, its your society – if there is more we could do or should change come and join us with your ideas and energy!

HOW YOU CAN SUPPORT ISCB

Dontate Now!

ANNA TRAMANTANO FUND

The goal of the Anna Tramontano Fellowship Fund is help reduce the financial burden to the students who are offered these internships by providing travel support. We hope that by providing financial support, reducing costs to the PIs, we will be able to increase the number of internships offered in a given year.

STUDENT FELLOWSHIP CAMPAIGN

YOU can make a difference in the future of computational biology and bioinformatics by supporting tomorrow’s researchers. By donating to ISCB student fellowships, you are investing in the future of our science..

GENERAL RESOURCES FUND

ISCB delivers valuable information about training, education, employment, and relevant news, and provide an influential voice on government and scientific policies that are important to our members and benefit the public. Your membership and generous support helps to make these activities possible.

SPONSOR MEMBERSHIP DUES OF MEMBERS FROM DEVELOPING COUNTRIES

Your contribution will help those in developing countries who cannot afford membership to join and benefit from ISCB.

https://www.iscb.org/support-iscb

The International Society for Computational Biology (ISCB) Innovator Award honors an ISCB scientist who is within two decades of his or her graduate degree completion and has consistently made outstanding contributions to the field of computational biology. The 2021 winner is Dr. Ben Raphael, Professor of Computer Science at Princeton University. He will receive his award and present a keynote address at the 2021 Joint Intelligent Systems for Molecular Biology (ISMB)/ European Conference on Computational Biology (ECCB) being held virtually on July 25-30, 2021.

Ben Raphael:
From Space Nut to Cancer Conqueror

Ben Raphael grew up in the Washington, DC area and was fascinated with science from a young age. His mother was a science teacher and nurtured a love of science in Raphael and his siblings. Raphael was first bitten by the "space bug," and he fondly recalls his two oldest brothers pooling their money to buy a telescope, which allowed Raphael and his family to enjoy many nights stargazing from their own yard. Raphael immersed himself in books about the space program, watched every shuttle launch, and frequented the nearby National Air and Space Museum. Eventually, Raphael was admitted to the Massachusetts Institute of Technology (MIT), where he pursued a major in mathematics and a minor in biology. Throughout his undergraduate coursework, he started to prefer mathematics courses that used abstract thinking and shifted away from fact-heavy biology courses. Raphael went on to pursue his PhD in Mathematics at the University of California, San Diego (UCSD) under the mentorship of Jim Agler. During his graduate studies, UCSD launched its Bioinformatics Graduate Program, and Raphael enrolled in a bioinformatics course offered by Pavel Pevzner, who had recently joined the UCSD faculty. This course was a major turning point for Raphael, as he recalled, "I found computational biology to be an amazing blend of the disciplines that I had pursued: mathematics, computer science, and biology. I was enamored by the huge potential of genome sequencing, as the human genome sequence had just been published and the mouse genome was well underway. Moreover, computational biology was such a broad discipline that I thought I would never be bored and could change my focus from mathematical and computational questions to biological questions depending on where my research led me."

Raphael is deeply appreciative of the mentorship he had early in his career. His PhD advisor Jim Agler not only taught him a great deal about mathematics, but also about not allowing one's ego or preconceived ideas to hamper the pursuit of truth. Raphael pursued his postdoctoral studies under Pevzner, who introduced him to computational biology and shaped how he approaches research questions to this very day. Raphael was introduced to the field of cancer genomics through his work with Colin Collins and Joe Gray during his postdoc, and these collaborators provided him with valuable guidance and support during his transition to an independent investigator. As a new assistant professor at Brown University, Raphael also received invaluable support from Rick Wilson and Elaine Mardis, who got him involved in The Cancer Genome Atlas (TGCA) project and other large-scale cancer projects. Raphael is now a tenured professor at Princeton, and he relishes the newfound freedom to pursue longer-term projects, while balancing the needs of his students and trainees, who are also building their publication records.

Raphael tries to apply lessons learned from his postdoc training under Pevzner, and he said, "My training strongly influences how I train my students to select research questions and conduct research. Biology is a vast discipline, and there are a wide range of problems where computational biologists can contribute. I learned from my postdoctoral advisor Pavel Pevzner the importance of clearly formulating a biological problem as a computational problem. In some cases, this formulation reduces the problem to one that is already solved – and perhaps solved with existing software. While there are many problems in biology that can benefit from the application of computational methods, we strive to find problems where there is a need for a new algorithm." Raphael is also strongly influenced by his mathematical training, which taught him that writing clear and precise problem statements and definitions can greatly clarify one's thinking about a complicated problem. He similarly trains his students to write a rigorous statement of the computational problem they are trying to solve, and to define their terminology carefully.

Raphael's scientific curiosity has been focused for several years on cancer genomics. He continues to be amazed by the mutational heterogeneity observed in different cancers, particularly the long tail phenomenon, for which only a few genes are frequently mutated in cohorts of cancer patients whereas a large portion of genes are rarely mutated. Raphael and his team developed methods to study mutation combinations in different pathways and networks that identified groups of genes that were more frequently mutated. He noticed that this method worked better for some cancers, like glioblastoma but did not work consistently across cancer types, and he believes these differences may be due to limitations of current sequencing methods and available data for different tumor types.

Raphael considers single cell DNA sequencing technology as a powerful tool for improving how we visualize the complexities of cancer, but he also sees much work to be done in understanding how tumors develop and change in response to treatment. Advances in single cell and spatial sequencing technologies as well as extensions of these methods to measure multiple parameters in parallel are providing more detailed insights into cancer cell biology and tumor heterogeneity. Raphael also sees the benefits of applying CRISPR technology to biological models, which has enabled analysis of interactions between somatic mutations and CRISPR gene knockouts in cancer cell lines that were otherwise undetected in tumor specimens. In 2020, Raphael also came to appreciate the power of these technologies for studying the immune system in the context of SARS-CoV-2 infection and COVID-19, and how these studies can be applied to vaccine development.

Raphael has been recognized for his research contributions throughout his career, including a Sloan Postdoctoral Fellowship (2002-2004), a Burroughs Wellcome Fund CAREER award at the Scientific Interface (2005), a Sloan Research Fellowship (2010) and an NSF CAREER award (2011-2017). He is considered a leader in algorithmic computational cancer biology research and his work has been published in top-tier scientific and computational biology journals. Raphael has developed several widely used algorithms that include THetA and AncesTree algorithms for analyzing mixtures of cancer cells, Dendrix and Multi-Dendrix algorithms for analyzing mutually exclusive mutations, and the HotNet algorithm for network analysis of cancer mutations.

Raphael has served the greater computational biology community in many ways, including working on the steering committees for the RECOMB Satellite Workshop on Computational Cancer Biology (2007-present) and the RECOMB Satellite Workshop on Massively Parallel Sequencing (2012-present). He has served on the program committees for ISMB, RECOMB, PSB, and many other conferences and has helped to organize research programs at UCLA, Bertinoro, the Simons Institute for the Theory of Computing, and other venues. Raphael has also reviewed grant proposals for NSF and NIH for most years since 2008. He is a key contributor to The Cancer Genome Atlas (TCGA) and International Cancer Genome Consortium (ICGC) projects and has taken on leadership roles in these projects.

Raphael is honored, humbled, and grateful for recognition with the 2021 ISCB Innovator Award. As an ISCB Fellow, he participated in the selection of new Fellows this year and came to appreciate the number of exceptional computational biology researchers being considered for recognition as a Fellow or for an ISCB award. Raphael is deeply grateful for his students and postdoctoral fellows who have worked hard and contributed to the success of many research projects. He is also thankful for the unwavering support of his wife and children through the many phases of his career.

International Society for Computational Biology (ISCB) recognizes a leader in the fields of computational biology or bioinformatics annually with the Accomplishments by a Senior Scientist Award. This is the highest award bestowed by ISCB in recognition of a scientist's significant research, education, and service contributions. Peer Bork, Director of EMBL Heidelberg (Scientific Activities), is being recognized with the 2021 Accomplishment by a Senior Scientist Award. He will receive his award and present a keynote address at the 2021 Joint Intelligent Systems for Molecular Biology (ISMB)/ European Conference on Computational Biology (ECCB) being held virtually on July 25-30, 2021.

Peer Bork

From Behind the Wall to the Microbiome

Peer Bork grew up in Berlin, East Germany before the fall of the Berlin Wall. Bork was interested in math as a young student and his math teacher encouraged him to join the chess club and compete in Math Olympiad, for which he eventually competed at a national level. Bork was most interested in logic because he enjoyed deducing mathematical concepts, and his early interest in math helped him to gain entry into a specialized math school for 9th-12th class. He was also a consummate reader and devoured books that explained biological phenomena like photosynthesis. Bork considered studying science as a viable career path, as he recalled, “I was always a curious person that used analytical thinking, and having grown up in East Germany, science was an area where I hoped that I could stick to facts with limited impact of political propaganda.” He attended the specialized math school in the early 1980’s, where he was first exposed computer programming through training on a Russian computer that was nearly the size of a car. Soon after, PCs were available in East Germany, and Bork had his first experience using computation to solve a biological problem as a young graduate student at the University of Leipzig. He said, “In a practicum during my biochemistry studies, I successfully optimized the commercial production of certain NADH-dependent dehydrogenases in a fermenter by computationally simulating reaction equations.” This experience helped him develop a project for his computational diploma (equivalent to a master’s degree) work in 1987, in which he worked to understand the evolution of enzyme cofactor binding domains in the context of substrate binding and turnover. He recalled, “For this I had to collect sequences of those enzymes, search emerging sequence databases, align them using early multiple alignment tools, and extend my mini-dataset by doing homology searches using a self-designed and self-coded (with a colleague) sequence pattern approach. The respective research field around sequence analysis was still small, but the databases expanded rapidly, and it was enjoyable to get to biological novelty quickly by using homology inferences (e.g., binding site prediction), identifying novel protein domains, or broadening existing ones using sequence signatures. It was not uncommon to get results sufficient for a good scientific paper within a week or so, and as a byproduct, one could learn a lot about molecular biology while reading the papers around the published protein sequences. I was fascinated by the independent evolution of such domains, and I shifted focus from enzymatic domains to more mobile ones to decipher the modular LEGO principle of building blocks for protein function. I stored the domains I discovered and/or described in a self-made database. This was rewarding and efficient, and I soon had enough material to be able to finish my PhD in 1.5 years. With this experience, I was already an expert and pioneer in a quickly

expanding research field with a high impact on biological research.” Bork’s PhD experience has shaped his selection of research topics, as he prefers to tackle nascent research areas for which little is known, and he takes a more data-driven rather than hypothesis-driven approach, thus freeing him of lofty expectations of experimental outcomes.

Bork credits much of his development into an independent researcher to his mentorship under his PhD supervisor Jens Reich (Berlin). He recounted, “When I joined his group in 1988, he was one of the leaders of the political underground movement in East Germany, shortly before the wall came down. He was under constant surveillance by the “Stasi,” and it was unclear whether he would end up in prison. He never made a fuss about his political standing, and at work he encouraged and helped me without micromanagement. A couple of years later, he was a runner-up for the German Federal Presidency. He treated everybody equally, was a knowledgeable and engaging supervisor and supported me, even during unification, when everyone at my institute lost their jobs and had to re-apply for the few new positions.” Reich continued to mentor Bork and other students despite his political duties as a member of the German Parliament and other pursuits, including writing essays for newspapers and authoring non-scientific books. Bork also valued the academic guidance that grew out of his work with Russell Doolittle, a world-renowned evolutionary biologist and biochemist at the University of California, San Diego, and said, “[Doolittle’s] enthusiasm, wisdom and focus on important things (for him), as well as his use of storytelling in science made a deep impression on me and others, and positively influenced my social skills and devotion to science.”

Bork completed his Habilitation in 1995 at Humboldt University in Berlin. He had concurrently joined EMBL Heidelberg in 1991, became Group Leader there in 1995, was promoted to Head of a unit (equivalent to department) in 2001, served additionally as Strategic Head of Bioinformatics since 2011 and is director of the Heidelberg site since 2020. Bork has made many meaningful contributions to bioinformatics, particularly through his early work on protein domains (SMART database), genome analysis of higher eukaryotes, work on methods for analysis of mutation data (PolyPhen) and large-scale phylogeny (iToL), as well as inventing several methods for inferring gene/protein networks (STRING database) and analysis of drugs and adverse reactions (STITCH and SIDER), and his recent pioneering microbiome research. Bork continues to be fascinated with this field, and said, “I moved research subfields a few times but got stuck on microbiomes for more than 15 years, mostly focusing on the human gut microbiome. I witnessed the very beginning of a quickly expanding field and have seen it progress to medical applications. I believe that the progress of the gut microbiome research towards improving human health can be paralleled by global microbiomics towards planetary health and this is a fascinating thought. It seems possible to get a census and understanding of molecular and cellular functions and their evolution for our entire planet. This might enable a much better evolutionary understanding of functions and help in the development of applications for biotechnology, but also towards solving societal questions like antibiotic resistance and general sustainability. I’m also fascinated by the ongoing scientific revolution in structural biology towards high resolution structures of entire cells, enabled by cryoEM technology. This will be yet another qualitatively new baseline understanding with plenty of practical applications.”

Like many scientists, Bork has had his share of unexpected findings that have changed his perspective or research approach. Bork explained, “I found our discovery of enterotypes, that is the stratification of the human population into microbial community types surprising, as we could not really explain it, and I think, despite tons of hypotheses, still nobody can really explain this observation.

Other examples against my own expectation were phenotypic patterns that were strong enough to pinpoint molecular mechanisms, for example medical drug side effects we could use for drug target identification, or predictions of which human-targeted drugs also impact the gut microbiome. Those findings did not change research strategies though, just encouraged me to remain open-minded in pursuing research.” He has published over 600 manuscripts, many of which are highly cited, and several of his web resources have stood the test of time, including, SMART, STRING, eggnog, SIDER, and iToL, due to an international network of researchers maintaining and further developing these, often led by group alumni.

Bork has supported the bioinformatics community in other capacities, including serving as a Senior Editor of Molecular Systems Biology and an Editorial Advisory Board Member of PLOS Computational Biology and a reviewer for interdisciplinary journals including Science and Cell. He has organized numerous EMBO courses and has remained dedicated to nurturing young scientists, for which he was recognized with the 2008 Nature award for mentoring in science. His own training under Reich has shaped him into a mentor that encourages students to explore different fields, with a focus on contextualizing these findings with other observations. Bork considers it important to share in strategic aspects of projects and encourages students to chart their own paths and present their work to the greater scientific community.

Bork has built his scientific career on exploring different subfields and methods, and he greatly appreciates his recognition with the 2021 Accomplishment by a Senior Scientist Award as it is conferred by his bioinformatics peers for his many varied contributions to the field.

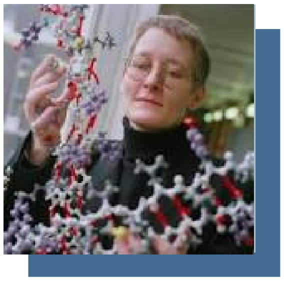
THANK YOU TO OUR GENEROUS DONORS

Jesus Galaz-Montoya
Emily Kawabata
Kevin Cohen
Nilson Da Rocha Coimbra
Dr. Lukeman Shittu
Boyang Ji
Rita Stack
Khalid Mahmood
Lawrence Hunter
Achille Zappa
Didier Barradas-Bautista
Clare Sansom
Didier Barradas-Bautista
Madhumita Bhattacharyya
Peter Ebert
Prashanth Suravajhala
Jyothi Thimmapuram
Jennifer Wilson
Roland Dunbrack
Bruno Fosso
Matteo Schiavinato
Lucy Forrest
Hrishikesh Deshmukh
Travis Johnson
Brent Cochran
Pier Luigi Martelli

2021 OUTSTANDING CONTRIBUTIONS TO ISCB AWARD

TERESA ATTWOOD

The Outstanding Contributions to the International Society for Computational Biology (ISCB) Award was initiated in 2015 to recognize members who have made beneficial and lasting contributions to the Society through their leadership, service, and educational work, or a combination of these three areas. Teresa (Terri) Attwood, Professor emerita at the School of Computer Science, The University of Manchester is the 2021 Outstanding Contributions to ISCB winner. She will receive her award at the 2021 Joint Intelligent Systems for Molecular Biology (ISMB)/ European Conference on Computational Biology (ECCB) being held virtually on July 25-30, 2021.



Teresa Attwood

A Voice for Bioinformatics Education

Attwood has spent much of her career as a champion of the bioinformatics education community. After completing her PhD in Biophysics at the University of Leeds in just two years, she was awarded a prestigious Royal Society University Research Fellowship (1993-2002) and was also a visiting fellow at the European Bioinformatics Institute (EMBL-EBI). In 2001, she rose to Chair of Bioinformatics at the School of Computer Science at the University of Manchester. Attwood recognized the critical importance of bioinformatics education for the greater scientific community and coauthored one of the first bioinformatics textbooks with David Parry-Smith, as well as two other educational texts coauthored with Paul Higgs, and with Steve Pettifer and Dave Thorne.

Attwood is an esteemed ISCB member who has advocated for bioinformatics education through her years of service with ISCB and the greater bioinformatics and computational biology communities. Attwood first became aware of ISCB when she attended the 1997 ISMB meeting in Halkidiki, and she soon became a regular ISMB attendee, as it was one of the few meetings focused on bioinformatics. She was especially interested in incorporating bioinformatics education into ISMB and contributed to the one-day satellite meeting called the Workshops on Education in Bioinformatics (WEB) that launched in 2001.

She continued her bioinformatics education and training advocacy by serving as a member of the ISCB Education Committee and as an ISCB Board Member (2013-2016). During her service as a Board member, Attwood was also Chair of GOBLET (Global Organization for Bioinformatics Learning, Education and Training) and worked closely with Fran Lewitter to better coordinate the objectives and activities of these two organizations to meet the surging worldwide demand for bioinformatics training. They succeeded in incorporating bioinformatics education and training into the ISMB program through the formation of the Education Community of Special Interest (COSI) and brought bioinformatics tutorials to other conferences through the support of ISCB. Attwood acknowledges that Lewitter’s shared passion for bioinformatics education and her desire to work together harmoniously were essential to their shared success in advancing their bioinformatics and training initiatives.

Attwood is recently retired from the University of Manchester and has deeply appreciated her ISCB involvement. She said, “I valued my membership in ISCB for creating my first ‘bioinformatics home’, bringing opportunities to meet like-minded people and to become part of a community. These early experiences provided the springboard for embracing a hugely diverse worldwide community, learning about their bioinformatics training needs, their challenges, and their innovative solutions.

Those first steps paved the way for working with colleagues to create a variety of bioinformatics training materials; to create the GOBLET Foundation and establish the Education COSI; to build the foundations of the bioinformatics training strategy of ELIXIR (Europe's data infrastructure), and to contribute to the development of its training portal (TeSS) and its Train-the-Trainer program; and to become involved with many other bioinformatics training programmes and initiatives worldwide. Ultimately, these opportunities opened doors to work with high school teachers, and to create materials and resources to help plug gaps in their bioinformatics training needs. It has been immensely gratifying to be able to work with, and to learn from, such experienced, supportive, and cherished colleagues across these varied educational contexts. Engaging with them to steer training projects within international societies and foundations (ISCB, ISB, SEB, EMBnet, ELIXIR, GOBLET and H3ABioNet to name but a few) taught me a lot."

Attwood encourages junior scientists and trainees to seek out service opportunities both to broaden their horizons and to build their networks. She appreciates how involvement in professional societies like ISCB gave her valuable opportunities to serve on working groups, task forces, and committees, and urges other young scientists to get involved in areas that "stir their hearts." Attwood has deeply valued the experiences that arose from her service to ISCB, but she has most treasured the decades-long relationships that have been built on trust and mutual respect and continue to be of great benefit even in retirement.

18th Annual Conference

ROCKY 2021 Bioinformatics Conference

ROCKY MOUNTAIN BIOINFORMATICS

December 2 - 4, 2021

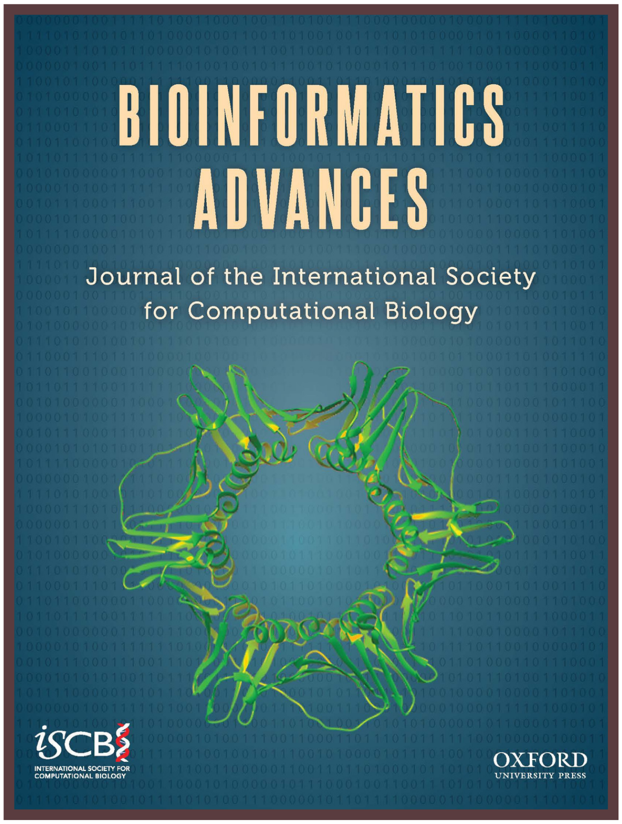
Viceroy Hotel
Snowmass Village
Colorado

CONFERENCE CHAIR:
LAWRENCE HUNTER, PH.D.
University of Colorado, Denver

GENERAL INFORMATION: rocky@iscb.org

www.iscb.org/rocky2021

ISCB INTERNATIONAL SOCIETY FOR COMPUTATIONAL BIOLOGY



BIOINFORMATICS ADVANCES

Journal of the International Society for Computational Biology

ISCB INTERNATIONAL SOCIETY FOR COMPUTATIONAL BIOLOGY

OXFORD UNIVERSITY PRESS

BARBARA ENGELHARDT

Each year the International Society for Computational Biology (ISCB) recognizes the achievements of an early to mid-career scientist with the Overton Prize. This prize honors the untimely death of Dr. G. Christian Overton, a respected computational biologist and founding ISCB Board member. The Overton Prize honors independent investigators who are in the early to middle phases of their careers and have made significant contributions to computational biology through research, teaching, and service.

ISCB is pleased to recognize Dr. Barbara Engelhardt, Associate Professor of Computer Science at Princeton University, as the 2021 winner of the Overton Prize. She will receive her award and present a keynote address at the 2021 Joint Intelligent Systems for Molecular Biology (ISMB)/ European Conference on Computational Biology (ECCB) being held virtually on July 25-30, 2021.

Barbara Engelhardt

A Winding Road that Leads to Statistics

Engelhardt grew up in New York City and recalled that her early encounters with math were rather frustrating. She had been placed in a remedial track in math until her fifth-grade teacher, Ms. Dorian, told her, “If I can’t read your work, I can’t grade you well.” From that moment, Engelhardt was able to express her mathematical prowess more clearly and excelled in upper-level mathematics classes through high school, including recognition with two coveted math awards. As a freshman at Stanford University, Engelhardt enrolled in the challenging honors math series, but she was less than enchanted with the heavy focus on theoretical math. She also took her first computer science class and recalled, “Everything clicked. It was less about proving things in math and more about logic and reasoning with math.” Engelhardt’s next mind-opening experience occurred when she took a machine learning class taught by Prof Daphne Koller, a new hire to the Computer Science department, that brought together many topics that interested her, including Bayesian networks and linear regression. Engelhardt went on to TA for Koller and complete an MS in Computer Science under her mentorship. She then took a position at the Jet Propulsion Laboratory (JPL) for two years, just as many of her peers were getting recruited to Google, which was a little-known startup at the time. Without a PhD, Engelhardt learned she would have limited opportunities for advancement at JPL, so she applied to grad school and landed at the University of California, Berkeley. She trained under Prof Michael Jordan, who not only guided her on her academic pursuits but taught her valuable lessons in mentorship and how to see “both the forest and the trees.” Engelhardt fondly recalls the famous group meetings that Jordan organized with his lab during which they would select a topic to learn about for several weeks and spend hours thinking through machine learning ideas and statistics concepts at great depth, even if they ultimately abandoned a concept they had considered applying to a research project. During grad school, Engelhardt immersed herself in statistics courses and came to really appreciate this area of mathematics because of the ability of statistical methods to explore data, find patterns, and solve important problems. She sought out a PhD project focused on a biological problem and collaborated with Prof Steven Brenner, ultimately leading to the completion of her dissertation on predicting protein molecular function in 2007. During her time at Berkeley, she also enjoyed interacting with Prof Monty Slatkin’s group, from which she learned of the fascinating connections between population genetics and statistics.

Engelhardt then had a brief stint at the nascent 23andMe and went on to be a postdoc at the University of Chicago under the advisement of Prof Matthew Stephens. She recalled, “[Stephens] constantly challenged me and the other people he mentored to understand our research from as many perspectives as possible to be able to best explain and teach the ideas to others, but also because he is a genuinely curious person.” During her postdoc, she performed research on new statistical approaches for association mapping for complex phenotypes and to identify population structure in genotype data. She considers her postdoc training as the time when she really learned how to think as a Bayesian statistician. Her foundational experiences as a grad student and postdoc honed her perspective on data science: The scientific question is the goal, and the methods used for the analysis of data should be as simple as possible while supporting the scientific goal as directly as possible.

Engelhardt launched her career as an independent researcher in 2011 when she took a position as a visiting research scientist at Duke University’s Biostatistics and Bioinformatics Department and was then hired as an assistant professor. She put her training to work as she sorted through what works and what does not work in Bayesian statistics. During this period, Engelhardt applied statistical models to complex phenotype association studies, differential gene expression analysis, and RNA sequencing (RNA-seq) data to better understand mechanisms of human disease. In 2014, Engelhardt joined the Computer Science Department at Princeton University, and she received tenure there in 2018. She has built a research program focused on developing statistical models and machine learning methods to analyze biomedical data, with a focus on identifying and characterizing complex associations, sequential decision making, and predicting the effects of perturbations in single-cell data, human cohorts, and medical record data. With her group, she has developed many valuable methods for analyzing and understanding single-cell genomic data, including a scalable and robust approach to dimension reduction using a Gaussian process latent variable model (GPLVM) with t-distributed residuals. Engelhardt has also led several large scale multi-disciplinary collaborations, including making foundational contributions to the Genotype-Tissue Expression (GTEx) Consortium and working with the Hospitals of the University of Pennsylvania to develop models for real-time hospital patient data, including vital signs and lab results, that can forecast these values several days in advance. Throughout her research, she has sometimes come upon negative results that lead her projects in different directions, including a recent observation that she could not really detect differences in outcome between black and white hospitalized COVID-19 patients but did find a five-year average age gap between these cohorts. She has come to value negative findings in a different way and said, “But instead of tossing the work, I think “Well, that’s interesting. I wonder why our results don’t match common knowledge in this domain. What does this negative result mean?” This thought process has led my group to some of our best work. These stories take a long time to play out sometimes, much to the frustration of the students working on them, but they are often worth the investment. Also, sometimes these follow up questions don’t require new tailor-made models and methods to find the source of the result; instead, asking for feedback from other scientists and being clever about how to test alternative hypotheses is the most insightful way forward. My favorite research directions are ones in which every dangling string is pulled – whether for methods development, biological questions, or hypothesis testing.”Engelhardt has expanded her research scope dramatically as an established PI, which she attributes to

having students who are interested in different biological problems. She said, “The wonderful thing about working in statistics and machine learning is that it is possible to work on problem domains that you haven’t tackled before by finding the right collaborator who is patient with your learning process throughout the collaboration. This means that I’ve been able to take advantage of students’ eagerness to work in medical data records, sociology, neuroscience, bioengineering, and psychology because we have found great collaborators and the students to drive those relationships.”

Engelhardt has been recognized for her rigorous and creative statistical approaches with several awards and recognitions, including an NSF CAREER Award and Sloan Faculty fellowship. As a PI, she most treasures her work in mentoring students and postdocs, and she has adapted the positive experiences she had as a trainee to her mentoring approach, including treating each person as a unique individual and fostering independence as well as collaboration. Outside of the lab, she has served the computational biology and greater biomedical communities in several ways, including service as the Diversity & Inclusion Co-Chair for the International Conference on Machine Learning, being a member of NIH Advisory Committee to the Director Working Group on Artificial Intelligence, working as a co-organizer for numerous workshops and meetings, and serving as an associate editor for the Annals of Applied Statistics.

Engelhardt feels tremendously honored to be selected for the Overton Prize, especially since she looks to so many of the previous Overton Prize winners. She also acknowledges that the work she has been recognized for would not be possible without the difficult and creative work carried out by her students and postdocs.

ISCB CAREER CENTER

ENGAGE INFORM RECRUIT

REPRESENTING ORGANIZATIONS WORLDWIDE
START YOUR JOB SEARCH HERE!

FIND A JOB
ISCB MEMBERS HAVE COMPLIMENTARY ACCESS TO THE ISCB JOBS BOARD

POST A CV
ISCB MEMBERS GET FREE CV UPLOADS
NONMEMBERS MAY PARTICIPATE FOR $100 PER CV

POST A JOB
ISCB MEMBERS RECEIVE COMPLIMENTARY POSTINGS AND CV REPOSITORY ACCESS
NONMEMBERS CAN REGISTER & POST FOR $300 PER JOB POSTING

LOOKING FOR A STRONG JOB CANDIDATE?
ISCB'S CAREER CENTER IS THE PLACE TO START!

WWW.ISCB.ORG/CAREERCENTER

MAKE THE MOST OF ISCB

Whether you're a lifetime member of ISCB or have just become a member, the resources below will help you make your membership with ISCB work for YOU!

The International Society for Computational Biology (ISCB) is a scholarly society for advancing understanding of living systems through computation and for communicating scientific advances worldwide.

1. Apply!

First, visit online and fill out the member form - it takes less than five minutes and your membership bomces activated the MINUTE you hit the submit button!

- LOGIN and complete or update your member profile
- ACCESS members-only resources, such as the career center, ISCB tv,
- FIND a long list of upcoming conferences and events near you at discounted rates!

2. Get Connected!

Next, get connected to other poeple in the field, find your COSI and take yourself to the next level

- CONNECT with other members through the online database of other ISCB members (3,500+ connections
- KEEP UP ISCB news and events through the bi-weekly ISCB Buzz and quarterly online Newsletters
- FIND the COSI (Community of Special Interest) that best fits your specialty and interest through involvment in topically-focused collaborative communities

3. Get Involved!

Now, use your expertise and time to give back to your profession

- VOLUNTEER your time and get involded with conferences, reviewing submissions and using your interests and expertise to help guide society committtes!
- VOTE for the leadership of the society --- help shape the future!
- SUPPORT those in the filed broaden their involment and growth by donating to the society or helping to fund travel fellowships to help the next generation of scientsts!

https://www.iscb.org/become-a-member

ISCB INTERNATIONAL SOCIETY FOR COMPUTATIONAL BIOLOGY

virtual

ISMB/ECCB 2021

CONFERENCE PROGRAMME

Welcome to Virtual ISMB/ECCB 2021

On behalf of the organizing committee of ISMB/ECCB 2021 and the Board of Directors of the International Society for Computational Biology (ISCB) we wish you a very warm and appreciative welcome. Though we realize nothing replaces being in person, this new virtual landscape built on the success and lessons learned, is sure to help recreate what the ISMB/ECCB conference alliance has become synonymous with collaboration, fostering fresh dialogue, and providing innumerable learning opportunities all from the comfort of your sofa or desk chair. We will all miss the architecture and history of what would have been an amazing in-person experience in Lyon but this virtual gathering promises to be an inventive and thought-provoking conference for all attendees!

Creating the core of the scientific program are the ISCB's Communities of Special Interest (COSIs), enabling intensified community involvement and bolstering its reputation as a conference with a strong scientific and technical program, which showcases the best international developments in the field. ISMB/ECCB 2021 is showcasing 21 COSIs with major computational biology themes ensuring you can connect more easily to researchers sharing common interests and come together and listen to exciting new developments in your field. These communities each run their respective sessions (COSI tracks or workshops) as part of the conference. You will have the opportunity to attend any of these sessions, choosing the presentations of most interest to you, live or as on-demand sessions.

Each day of the conference includes outstanding keynote lectures, technical talks, talks from the published conference proceedings in Bioinformatics, additional published and unpublished talks thematically organized in the COSI tracks, a variety of workshops, special sessions, equal opportunities activities, a students organized symposium, a virtual exhibition hall, live poster presentation room, and fully interactive poster sessions. The structure is intended to bring a new energy and flow to the conference by centering it thematically around the vibrant ISCB COSIs. Further, with the COSIs more central to the conference, networking within and between the scientific communities is greatly enhanced.

All of the sessions will be on a predetermined broadcast schedule. You can browse the schedule at your leisure and even mark the talks that you are most interested in seeing. If you miss something, don't worry! You will be able to access this platform until November 30, 2021, and all of the talks (and the virtual poster hall) presented will be available on-demand to watch at your convenience.

As is the goal every year, ISMB/ECCB will aim to bring together scientists from computer science, molecular biology, mathematics, statistics and related fields, and to provide an intense multidisciplinary forum for disseminating the latest developments in bioinformatics/computational biology in a virtual environment.

The virtual platform of the conference will foster fresh dialogues, collaboration, and learning opportunities.

- *3 renowned Keynote speakers*
- *3 Keynote addresses from the 2021 ISCB Award Winners*
- *Training workshops and tutorials*
- *Student Council Symposium*
- *Live and on-demand sessions to benefit attendees from all time zones*
- *600+ scientific talks*
- *Live question and answer feature to engage with the speaker during sessions*
- *Live chat feature to engage with other participants within your session room*
- *Dedicated time for research presentation within the Research Exchange Forum (formerly Poster Hall)*
- *Ability to make new connections when utilizing the attendee profile and match maker features*
- *Schedule one-on-one time with speakers, poster presenters, exhibitors, and sponsors to learn more about their work, products, or services*
- *Exclusive access to the ISMB/ECCB 2021 on-demand repository of talks and poster presentations for viewing at your leisure after conference dates*

Though we realize nothing replaces trying to run across a convention center between sessions, ISCB is making every effort to create a virtual experience that mirrors an in-person experience but with less sore feet at the end of the day.

We want to acknowledge all the chairs of the Proceedings, COSIs, COVID-19, Technology Track, Travel Fellowship, Tutorials, and Student Council Symposium committees. Their dedication and leadership during this time has been invaluable in offering to you an insightful, relevant, and cutting-edge program.

We, of course, want to extend our appreciation to our conference sponsors and exhibitors for their ongoing support during these trying times. This year's virtual exhibition section will be a key feature for attendees to learn more about publishing opportunities, services, tools, and job openings.

Finally, we wish you all a great virtual conference experience! Enjoy ISMB/ECCB 2021!

Yours sincerely,

Marie-France Sagot

Rita Casadio

Jacques Van Helden

Conference Co-Chairs

Scientific Organizing Committee

CONFERENCE CHAIRS

CONFERENCE CO-CHAIR
Rita Casadio
University of Bologna
Italy

CONFERENCE CO-CHAIR
Marie-France Sagot
French Institute for Research in
Computer Science and
Automation (INRIA),
University of Lyon, France

CONFERENCE CO-CHAIR
Jacques Van Helden
Aix-Marseille Université (AMU),
Marseille, France

ISMB/ECCB 2021 STEERING COMMITTEE

Rita Casadio, Conference Co-chair, University of Bologna, Italy

Christophe Dessimoz, University of Lausanne; University College London; Swiss Institute for Bioinformatics, Switzerland

Bruno Gaeta, ISCB Treasurer, University of New South Wales, Australia

Janet Kelso, ISCB Conference Advisory Council Co-chair, Max Planck Institute for Evolutionary Anthropology, Germany

Diane E. Kovats, ISCB Chief Executive Officer, United States

Steven Leard, ISMB Conference Director, Canada

Teresa M. Przytycka, NCBI, NLM, NIH, United States

Thomas Lengauer, ISCB Past-President, Max Planck Institute for Informatics, Germany

Christine Orengo, ISCB President, University College London, United Kingdom

Pat Rodenburg, Conference Administrator, Canada

Marie-France Sagot, Conference Co-chair, Claude Bernard University; French Institute for Research in Computer Science and Automation (INRIA); University of Lyon, France

Torsten Schwede, ECCB Liaison, Biozentrum, University of Basel & SIB Swiss Institute of Bioinformatics Switzerland

Jacques Van Helden, Conference Co-chair, Aix-Marseille Université (AMU), France

PROCEEDINGS COMMITTEE

PROCEEDINGS CO-CHAIRS

Christophe Dessimoz, University of Lausanne; Swiss Institute for Bioinformatics, Switzerland
Teresa M. Przytycka, NCBI, NLM, NIH, United States

AREA CHAIRS

BIOINFORMATICS EDUCATION
Sarah L. Morgan, *EMBL-EBI, United Kingdom*
Russel Schwartz, *Carnegie Mellon University, United States*

BIOINFORMATICS OF MICROBES AND MICROBIOMES
Bernhard Renard, *Hasso Plattner Institute*
Hélène Touzet, CNRS, CRIStAL, France

BIOMEDICAL INFORMATICS
Maria Secrier, *University College London, United Kingdom*
Marinka Zitnik, *Harvard University, United States*

EVOLUTIONARY, COMPARATIVE, AND POPULATION GENOMICS
Dannie Durand, *Carnegie Mellon University, United States*
Wataru Iwasaki, *University of Tokyo, Japan*

GENOME PRIVACY AND SECURITY
Bonnie Berger, *Massachusetts Institute of Technology, United States*

GENOMIC SEQUENCE ANALYSIS
Can Alkan, *Bilkent University, Turkey*
Adam Phlilippy, *NIH, United States*

MACROMOLECULAR SEQUENCE, STRUCTURE, AND FUNCTION
Yann Ponty, CNRS/LIX, *Polytechnique, France*
Jinbo Xu , *Toyota Technological Institute at Chicago, United States*

REGULATORY AND FUNCTIONAL GENOMICS
Shaun Mahony, *Penn State, United States*
Yvan Saeys, *VIB Ghent, Belgium*

SYSTEMS BIOLOGY AND NETWORKS
Laurent Jacob, *CNRS, France*
Tamer Kahveci, *University of Florida, United States*

GENERAL COMPUTATIONAL BIOLOGY
Mohammed El-Kebir, *University of Illinois, United States*
Cagatay Turkay, *University of Warwick, United Kingdom*

Scientific Organizing Committee

COSI TRACK LEADS & ABSTRACT CHAIRS

3D-SIG: STRUCTURAL BIOINFORMATICS AND COMPUTATIONAL BIOPHYSICS

Iris Antes, *Technical University of Munich, Germany*
Douglas Pires, *The University of Melbourne, Australia*
Rafael Najmanovich, *University of Montreal, Canada*

BIOINFO-CORE

IMadelaine Gogol, *Stowers Institute, United States*
Rodrigo Ortega Polo, *Agriculture and Agri-Food Canada*
Alberto Riva, *University of Florida, United States*

BIO-ONTOLOGIES

Tiffany Callahan, *University of Colorado Denver, United States*
Robert Hoehndorf, *King Abdullah University of Science & Technology, Saudi Arabia*

BOSC: BIOINFORMATICS OPEN SOURCE CONFERENCE

Peter Cock, *James Hutton Institute, United Kingdom*
Chris Fields, *University of Illinois, United States*
Nomi L. Harris, *Lawrence Berkeley National Laboratory, United States*
Karsten Hokamp, *Trinity College Dublin, Ireland*

BIOVIS: BIOLOGICAL DATA VISUALIZATIONS

Danielle Albers Szafir, *University of Colorado at Boulder, United States*
Jan Byška, *Masaryk University, Czech Republic*
Helena Jambor, *TU Dresden, Germany*
Cagatay Turkay, *University of Warwick, United Kingdom*

CAMDA: CRITICAL ASSESSMENT OF MASSIVE DATA ANALYSIS

David Kreil, *Boku University Vienna, Austria*
Joaquin Dopazo, *Fundación Progreso y Salud, Spain*
Paweł P Łabaj, *Austrian Academy of Sciences, and Jagiellonian University, Poland*
Wenzhong Xiao, *Harvard Medical School, United States*

COMPMS: COMPUTATIONAL MASS SPECTROMETRY

Wout Bittremieux, *University of California San Diego, United States*
Isabell Bludeau, *Max Planck Institute of Biochemistry, Germany*
Lindsay Pino, *University of Pennsylvania, United States*
Timo Sachsenberg, *University of Tübingen, Germany*

EDUCATION: COMPUTATIONAL BIOLOGY AND BIOINFORMATICS EDUCATION AND TRAINING

Annette McGrath, *Australian Commonwealth Scientific and Industrial Research Organisation (CSIRO), Australia*
Patricia M. Palagi, *SIB Swiss Institute of Bioinformatics, Switzerland*
Russell Schwartz, *Carnegie Mellon University, United States*

EVOLCOMPGEN: EVOLUTION & COMPARATIVE GENOMICS

Edward L. *Braun, University of Florida, United States*
Janani Ravi, *Michigan State University, United States*
Giltae Song, *Pusan National University, Korea*

FUNCTION: INCORPORATING CAFA 4: GENE AND PROTEIN FUNCTION ANNOTATION

Iddo Friedberg, *Iowa State University, United States*
Casey S. Greene, *University of Colorado, United States*
Sean D Mooney, *University of Washington, United States*
Kimberly Reynolds, *University of Texas Southwestern Medical Center, United States*
Mark Wass, *University of Kent, United Kingdom*
Predrag Radivojac, *Northeastern University, United States*

HITSEQ: HIGH THROUGHPUT SEQUENCING ALGORITHMS & APPLICATIONS

Can Alkan, *Bilkent University, Turkey*
Ana Conesa, *University of Florida, United States*
Francisco M. De La Vega, *Stanford University, United States*
Dirk Evers, *Dr. Dirk Evers Consulting, Germany*
Gang Fang, *Mount Sinai School of Medicine, United States*
Kjong Lehmann, *ETH-Zürich, Switzerland*
Layla Oesper, *Carleton College, United States*
Gunnar Rätsch, *ETH-Zürich, Switzerland*

IRNA: INTEGRATIVE RNA BIOLOGY

Athma Pai, *University of Massachusetts Medical School, United States*
Klemens Hertel, *UC Irvine, United States*
Michelle Scott, *University of Sherbrooke, Canada*
Yoseph Barash, *University of Pennsylvania, United States*

MLCSB: MACHINE LEARNING IN COMPUTATIONAL AND SYSTEMS BIOLOGY

Christoph Lippert, *University of Potsdam, GermanyAnshul Kundaje, Stanford University, United States*
Gabriele Schweikert, *Dundee University, Scotland*

MICROBIOME

Aaron Darling, *University of Technology Sydney, Australia*
Alice McHardy, *Helmholtz Centre for Infection Research, Germany*
Alexander Sczyrba, *Bielefeld University, Germany*
Thea Van Rossum, *EMBL Heidelberg, Germany*
Zhong Wang, *Joint Genome Institute, United States*

NETBIO: NETWORK BIOLOGY

Martina (Tina) Kutmon, *Maastricht University, Netherlands*
Tijana Milenkovic, *University of Notre Dame, United States*
Natasa Przulj, *ICREA Research Professor, Catalan Institution for Research and Advanced Studies (ICREA); Group Leader, Barcelona Supercomputing Center; Professor of Computer Science, University College London.*

REGSYS: REGULATORY AND SYSTEMS GENOMICS

Shaun Mahony, *Penn State University, United States*
Anthony Mathelier, *University of Oslo, Norway*
Lonnie Welch, *Ohio University, United States*
Judith Zaugg, *EMBL, Germany*

Scientific Organizing Committee

COSI TRACK LEADS & ABSTRACT CHAIRS

SYSMOD: COMPUTATIONAL MODELING OF BIOLOGICAL SYSTEMS

Laurence Calzone, *Institut Curie, France*
Claudine Chaouiya, *Aix-Marseille Université, France*
Andreas Dräger, *University of Tübingen, Germany*
María Rodríguez Matínez, *IBM Research Europe, Switzerland*
Juilee Thakar, *University of Rochester Medical Center, United States*

TEXT MINING

Cecilia Arighi, *University of Delaware, United States*
Lars Juhl Jensen, *University of Copenhagen, Denmark*
Robert Leaman, *NCBI/NLM/NIH, United States*
Zhiyong Lu, *NCBI/NLM/NIH, United States*

TRANSMED: TRANSLATIONAL MEDICINE INFORMATICS & APPLICATIONS

Irina Balaur, *University of Luxembourg*
Wei Gu, *University of Luxembourg*
Venkata Satagopam, *University of Luxembourg*
Mansoor Saqi, *Kings College London, United Kingdom*
Maria Secrier, *University College London, United Kingdom*

COVID-19 ABSTRACT COMMITTEE

Thomas Lengauer, *Max Planck Institute for Informatics, Germany*
Shoshana Wodak, *VIB-VUB Center for Structural Biology, Belgium*
Rita Casadio, *University of Bologna, Italy*
Christophe Dessimoz, *University College London, United Kingdom*
Bruno Gaeta, *The University of New South Wales, Australia*
Wataru Iwaskai, *The University of Tokyo, Japan*
Janet Kelso, *Max Planck Institute for Evolutionary Anthropology, Germany*
Stephen MacKinnon, *Cyclica, Canada*
Christine Orengo, *University College London, United Kingdom*
Teresa Przytycka, *National Center of Biotechnology Information, NLM, NIH, United States*
Sushmita Roy *University of Wisconsin-Madison, United States*
Marie-France Sagot, *Claude Bernard University; French Institute for Research in Computer Science and Automation (INRIA); University of Lyon, France*
Russell Schwartz, *Carnegie Mellon University, United States*
Jinbo Xu, *Toyota Technological Institute at Chicago, United States*

SPECIAL SESSIONS

Co-Chair: Céline Brochier-Armanet, *Université de Lyon, France*
Co-Chair: Yves Moreau, *KU Leuven, Belgium*

VARI: VARIANT INTERPRETATION

Emidio Capriotti, *University of Bologna, Italy*
Hannah Carter, *University of California, San Diego, United States*
Antonio Rausell, *Imagine Institute for Genetic Diseases, France*

GENERAL COMPUTATIONAL BIOLOGY

Xin Gao, *King Abdullah University of Science and Technology (KAUST), Saudi Arabia*
Xuegong Zhang, *Tsinghua University, China*

TECHNOLOGY TRACK COMMITTEE

Chair: Hagit Shatkay, *University of Delaware, United States*

TUTORIALS

Chair: Annette McGrath, *Commonwealth Scientific and Industrial Research Organisation (CSIRO), Australia*
Co-chair: Michelle Brazas, *Ontario Institute for Cancer Research, Canada*
Co-chair: Patricia M. Palagi, *SIB Swiss Institute of Bioinformatics, Switzerland*

Distinguished Keynote Presentations

SUNDAY, JULY 25, 16:20 - 17:20 UTC

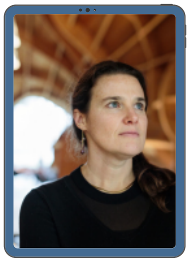
Rodrigo A. Gutierrez

Universidad Catolica de Chile

Phylogenomics and Systems Biology approaches reveal conserved adaptive processes in Atacama Desert plants

Introduced by: Marie-France Sagot, Conference Co-Chair

MONDAY, JULY 26, 16:20 – 17:20 UTC



ISCB Overton Prize Keynote

Barbara Engelhardt

Princeton University

Cells in Space: Methods to investigate local neighborhoods of cells

Introduced by: Rita Casadio, Conference Co-chair

TUESDAY, JULY 27, 16:20 – 17:20 UTC

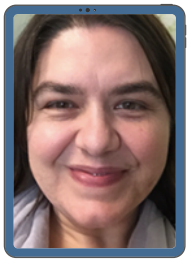
Eduardo Rocha

Institut Pasteur

Cosmos from chaos: how intra-genomic conflicts and horizontal transfer drive genome evolution

Introduced by: Jacques Van Helden, Conference Co-chair

WEDNESDAY, JULY 28,16:20 – 17:20 UTC



Kate Jones

University College London

Our Planet, Our Health - Ecosystem approaches to forecasting zoonotic diseases

Introduced by: Thomas Lengauer, ISCB Past-President

THURSDAY, JULY 29, 16:20 – 17:20 UTC

ISCB Innovator Award Keynote

Ben Raphael

Lewis-Sigler Institute, Princeton University

Quantifying Tumor Heterogeneity across Time and Space

Introduced by: Christine Orengo, ISCB President

FRIDAY, JULY 30, 15:20 – 16:20 UTC

ISCB Accomplishments by a Senior Scientist Award Keynote

Peer Bork

EMBL Heidelberg

Analyzing microbes in us and on our planet

Introduced by: Martin Vingron, ISCB Awards Committee Chair

Exhibitors & Recruiters

International Society for Computational Biology

www.iscb.orgThe International Society for Computational Biology (ISCB) was the first and continues to be the only society representing computational biology and bioinformatics worldwide. ISCB serves a global community of over **3,000** scientists dedicated to advancing the scientific understanding of living systems through computation by:

- convening the world's experts and future leaders in top conferences
- partnering with publications that promote discovery and expand access to computational biology and bioinformatics
- delivering valuable information about training, education, employment, and relevant news
- providing an influential voice on government and scientific policies that are important to our members

ISCB has three official journals – OUP Bioinformatics, OUP Bioinformatics Advances and F1000Research ISCB Community Journal, and has affiliations in place with several other publications for the benefit of our members.

www.iscb.org

ISCB Student Council

ISCB Student Council is an international network of young researchers in the broader disciplines of Computational Biology. SC provides opportunities for networking, career enhancement, and skills development for the next generation of Computational Biology leaders. The SC Symposium is organized as a part of the annual ISMB conference with student presentations, keynotes, panel discussions, and a poster session. This year, the symposium edition is the 17th Student Council Symposium. The booth will include the highlights of our recent virtual conference (winners, new experiences, and results of the RSGs leadership meeting).

www.iscbsc.org

BioCyc/SRI International

Pathway Tools is a comprehensive bioinformatics software package that spans enterprise genome data management, systems biology, and omics data analysis. The software has been licensed by more than 11,000 groups, and it powers the BioCyc.org website. It provides extensive search and visualization tools; computational inferences such as metabolic reconstruction; browsers for genomes, metabolic networks, and regulatory networks; transcriptomics and metabolomics data analysis, comparative analysis, and metabolic route search; sequence search and alignment.

BioCyc is a collection of 18,000 Pathway/Genome Databases (PGDBs) for model eukaryotes and for thousands of microbes, plus software tools for exploring them. BioCyc is an encyclopedic reference that contains curated data from 130,000 publications. BioCyc integrates genome data with a comprehensive body of additional data including metabolic reconstructions, regulatory networks, protein features, orthologs, gene essentiality, and atom mappings. BioCyc contains a vast set of bioinformatics tools including browsers for genomes, metabolic networks, and regulatory networks; transcriptomics and metabolomics data analysis, comparative analysis, and metabolic route search; sequence search and alignment.

www.biocyc.org and www.pathwaytools.com

EMBL's European Bioinformatics Institute (EMBL-EBI)

EMBL's European Bioinformatics Institute (EMBL-EBI) is a global leader in the storage, analysis and dissemination of large biological datasets.
We help scientists realise the potential of big data by enhancing their ability to exploit complex information to make discoveries that benefit humankind. We are at the forefront of computational biology research and we offer a wide range of bioinformatics training.

We are part of the European Molecular Biology Laboratory and are based just outside Cambridge, in the United Kingdom.

www.ebi.ac.uk/

Exhibitors & Recruiters

PerMedCoE: HPC/Exascale Centre of Excellence in Personalised Medicine

Personalised Medicine (PerMed) opens unexplored frontiers to treat diseases at the individual level combining clinical and omics information. However, the performances of the current simulation software are still insufficient to tackle medical problems such as tumour evolution or patient-specific treatments. The challenge is to develop a sustainable roadmap to scale-up the essential software for the cell-level simulation to the new European HPC/Exascale systems.

Simulation of cellular mechanistic models are essential for the translation of omic data to medical relevant actions and these should be accessible to the end-users in the appropriate environment of the PerMed-specific big confidential data. The goal of PerMedCoE is to provide an efficient and sustainable entry point to the HPC/Exascale-upgraded methodology to translate omics analyses into actionable models of cellular functions of medical relevance. It will accomplish so by

- optimising four core applications for cell-level simulations to the new pre-exascale platforms;
- integrating PerMed into the new European HPC/Exascale ecosystem, by offering access to HPC/Exascale-adapted and optimised software;
- running a comprehensive set of PerMed use cases; &
- building the basis for the sustainability of the PerMedCoE by coordinating PerMed and HPC communities, and reaching out to industrial and academic end-users, with use cases, training, expertise, and best practices.

The PerMedCoE cell-level simulations will fill the gap between the molecular- and organ-level simulations from the Centres of Excellence CompBioMed and BioExcel, with which this proposal is aligned at different levels. It will connect methods developers with HPC, HTC and HPDA experts (at the Centres of Excellence POP and HiDALGO). Finally, the PerMedCoE will work with biomedical consortia (i.e. ELIXIR, LifeTime initiative) and pre-exascale infrastructures (BSC and CSC), including a substantial co-design effort.

permedcoe.eu/

Nature Research

Nature Portfolio’s high-quality products and services across the life, physical, chemical and applied sciences are dedicated to serving the scientific community. Our journals publish some of the world's most significant scientific discoveries. The portfolio includes Nature and many more research and reviews titles such as Nature Computational Science. Nature Portfolio also offers a range of researcher services. For information on the portfolio please visit nature.com and to discover more about our new title Nature Computational Science please visit the journal homepage or speak to our Editor attending the conference, Ananya Rastogi, via the booth appointment scheduler or email.

www.nature.com

Oxford University Press

Oxford University Press publishes a range of computational biology journals, including Bioinformatics, Bioinformatics Advances, GigaScience, Nucleic Acids Research, NAR Genomics and Bioinformatics, Database, Briefings in Bioinformatics, Briefings in Functional Genomics, and more. Cailin Deery, the publisher for Bioinformatics is exhibiting on behalf of OUP during ISMB this year.

Bioinformatics publishes the highest quality scientific papers and review articles with its main focus is on new developments in genome bioinformatics and computational biology. To say hello, ask a question, provide feedback or otherwise, please don’t hesitate to get in touch through the conference scheduling tool.

academic.oup.com/BIOINFORMATICS

Exhibitors & Recruiters

Harvard Medical School Department of Biomedical Informatics

The Harvard Medical School Department of Biomedical Informatics offers a variety of opportunities to increase your knowledge base and skill set in the application of quantitative principles to biomedical discovery. Come learn about our educational programs which include a Master's, PhD, and Summer Institute and hear about our postdoctoral fellowships, faculty positions and other career opportunities.

Visit our booth to learn more about educational and career opportunities during the Research Exchange Forum (15:20 - 16:20 UTC) Monday 26 – Thursday 29.

For more information please visit: http://dbmi.hms.harvard.edu

dbmi.hms.harvard.edu

The German Network for Bioinformatics Infrastructure - de.NBI

The German Network for Bioinformatics Infrastructure (de.NBI) is a national, academic and non-profit infrastructure supported by the German Ministry of Education and Research (BMBF). The network consists of eight Service Centers which are specialized in different omics fields assuring excellent services and high level of expertise. With its wide range of bioinformatics know-how, the de.NBI network is aimed to deliver high standard bioinformatics services, comprehensive training, powerful compute capacities (de.NBI Cloud) as well as connections to industrial companies in Germany and Europe.

The de.NBI tool portfolio comprises over 160 services ranging from databases and stand-alone tools to complete workflows for the processing and analysis of omics data. In the field of training, de.NBI offers tailor-made training courses, webinars, summer schools and online courses on experimental data analysis which enable researchers in the life sciences to transform their raw data into actual results. Training courses are aimed at application users in life sciences as well as bioinformaticians and developers. The de.NBI Cloud provides an excellent solution to enable integrative analyses and the efficient use of data as virtual machines and open stack in research and application. Researchers from the life sciences in Germany can use the de.NBI Cloud free of charge. With its wide range of bioinformatics expertise and renowned partner institutions, the de.NBI network guarantees the delivery of high standards bioinformatics services that contributes to the advancement of bioinformatics research in Germany and Europe.

www.denbi.de/

F1000Research

F1000Research enables scientists and scholars to publish their research rapidly, openly, and transparently via an author-centric platform. We publish research across all academic disciplines and in multiple formats, including original articles, data notes, software tool articles and method articles. F1000Research operates a unique post-publication open peer review process, enabling authors to engage with their reviewers transparently, whilst also making the research available to a global audience as quickly as possible.

f1000research.com

GOBLET

GOBLET is an international organisation with the mission to cultivate a global community of bioinformatics trainers who support learning, education and training. GOBLET's mission was defined under the vision that there is a clear need to harmonise bioinformatics training activities and to unite, inspire, and equip bioinformatics trainers worldwide. Towards this, GOBLET collaborates with national and international bioinformatics organisations. Relevant activities include the initiation of a series of standards and guidelines, work on the definition of competencies, promotion of best practices, and providing high-quality resources for learning, education and training in bioinformatics and computational biology, on a global scale.

www.mygoblet.org

UCLA Medical Informatics Home Area

The Medical Informatics Home Area is UCLA's nexus for interdisciplinary training of the next generation of scientists involved in biomedical informatics and data science. UCLA provides a unique environment to bring together cutting-edge expertise and experience in a dynamic environment for graduate students engaged at the intersection of engineering, medicine, public health, and other related fields — and focusing on the goal of transforming modern healthcare through contemporary data-driven methods and tools.

Visit our booth to learn more!

biomedicalinformatics.ucla.edu/

MemVerge

As the world's enterprises accelerate their digital transformations, they discover that next-generation applications must deal with data that are bigger and faster at the same time, outstripping the capabilities of today's infrastructure. MemVerge's mission is to deliver a new architecture, called Big Memory Computing, that converges memory and storage, thereby removing the storage I/O bottleneck once and for all.

MemVerge's Memory Machine™ Software virtualizes heterogeneous memory hardware into a software-defined memory service that has both high capacity and high performance. MemVerge ZeroIO™ In-Memory Snapshot technology captures the state of running applications, and can be used for application roll-back, cloning and high availability. The results are new levels of productivity, performance, availability, and mobility for today's data-centric applications, both on-premises and in the cloud.

memverge.com/

ISCB Appreciates the Support of the Following Sponsors

ISCB ISMB ECCB 2021 • VIRTUAL

NIH National Institutes of Health
Office of Data Science Strategy

VE RI TAS
HARVARD
MEDICAL SCHOOL

DEPARTMENT OF
Biomedical Informatics

janssen Immunology
PHARMACEUTICAL COMPANIES OF Johnson & Johnson

de.NBI
GERMAN NETWORK FOR BIOINFORMATICS INFRASTRUCTURE

MemVerge

Schedule-at-a-glance
Sunday

Daily Schedule is Coordinated Universal Time or UTC

11:00	Sunday, July 25, Track Listing

11:00 - 15:30	**Workshop on Education for Bioinformatics (WEB2021)**
11:00 - 15:20	**3DSIG**
11:00 - 15:20	**Bio-Ontologies**
11:00 - 15:20	**HitSeq**
11:00 - 15:20	**TransMed**
11:00 - 14:00	**Special Session: Computational Biology going Green**
11:05 - 15:15	**Special Session: Representation learning in biology**

12:20	Programme Break
12:40	Sessions Continue
14:00	Programme Break
14:20	Sessions Continue
15:20	Research Exchange Forum includes Posters and Exhibitors / BoFs
16:20	ISMB/ECCB Distinguished Keynote: Rodrigo A. Gutierrez, Universidad Catolica de Chile Introduced by: Marie-France Sagot, Conference Co-Chair
17:20	Daily Closing Comments

Schedule-at-a-glance
Monday

Daily Schedule is Coordinated Universal Time or UTC

	Monday, July 26, Track Listing
10:00	ISCB Town Hall
11:00	

11:00 - 12:00	**HitSeq**
11:00 - 15:00	**3DSIG**
11:00 - 14:00	**Bio-Ontologies**
11:00 - 15:20	**BioVis**
11:00 - 15:20	**CompMS**
11:00 - 15:20	**EvolCompGen**
11:00 - 15:20	**NetBio**
11:00 - 15:20	**RegSys**
11:00 - 15:20	**TransMed**
11:00 - 15:30	**Education**

12:20	Programme Break
12:40	Sessions Continue
14:00	Programme Break
14:20	Sessions Continue
15:20	Research Exchange Forum includes Posters and Exhibitors / BoFs
16:20	ISCB Overton Prize Keynote: Barbara Engelhardt, Princeton University Introduced by: Rita Casadio, Conference Co-chair
17:20	Daily Closing Comments

Schedule-at-a-glance
Tuesday

Daily Schedule is Coordinated Universal Time or UTC

11:00 Tuesday, July 27, Track Listing

11:00 - 15:20	**HitSeq**
11:00 - 15:00	**3DSIG**
11:00 - 15:20	**NIH/ODSS**
11:00 - 15:20	**BioVis**
11:00 - 15:20	**CompMS**
11:00 - 15:20	**EvolCompGen**
11:00 - 15:20	**NetBio**
11:00 - 3:20	**RegSys**
11:00 - 15:20	**Special Session: New developments in AI for Integrating imaging and genomic data**
11:00 - 15:30	**Education**

12:20 Programme Break

12:40 Sessions Continue

14:00 Programme Break

14:20 Sessions Continue

ISCB Public Affairs and Policy Committee Special Session: Science Communication and Science Journalism

15:20 Research Exchange Forum includes Posters and Exhibitors / BoFs

16:20 ISMB/ECCB Distinguished Keynote:
Eduardo Rocha, Institut Pasteur
Introduced by: Jacques Van Helden, Conference Co-chair

17:20 Daily Closing Comments

Schedule-at-a-glance
Wednesday

Daily Schedule is Coordinated Universal Time or UTC

11:00	Wednesday, July 28, Track Listing

11:00 - 15:20	**MLCSB**
11:00 - 15:20	**CAMDA**
11:00 - 15:20	**Function**
11:00 - 15:20	**EvolCompGen**
11:00 - 15:20	**NIH/ODSS**
11:00 - 15:20	**RegSys**
11:00 - 15:20	**Microbiome**
11:00 - 15:20	**Special Session: Emerging gain-of-function mutations and their characterization by multi-omics network biology**
11:00 - 15:20	**TextMining**
11:00 - 15:20	**iRNA**

12:20	Programme Break
12:40	Sessions Continue
14:00	Programme Break
14:20	Sessions Continue
15:20	Research Exchange Forum includes Posters and Exhibitors / BoFs
16:20	ISMB/ECCB Distinguished Keynote: Kate Jones, University College London Introduced by: Thomas Lengauer, ISCB Past-President
17:20	Daily Closing Comments

Schedule-at-a-glance
Thursday

Daily Schedule is Coordinated Universal Time or UTC

11:00	Thursday, July 29, Track Listing

11:00 - 16:30	**iRNA**
11:00 - 15:20	**BOSC**
11:00 - 15:20	**General Computational Biology**
11:00 - 15:20	**MLCSB**
11:00 - 15:20	**SysMod**
11:00 - 15:20	**VarI**
11:00 - 15:20	**Function**
11:20 - 15:10	**MICROBIOME**
11:00 - 15:10	**CAMDA**

12:20	Programme Break
12:40	Sessions Continue

12:40 - 14:00	**Tools for Protein Analysis Hackathon**

14:00	Programme Break
14:20	Sessions Continue
15:20	Research Exchange Forum includes Posters and Exhibitors / BoFs
16:20	ISCB Innovator Award Keynote: Ben Raphael, Princeton University Introduced by: Christine Orengo, ISCB President
17:20	Daily Closing Comments

Schedule-at-a-glance
Friday

Daily Schedule is Coordinated Universal Time or UTC

Friday, July 30, Track Listing

11:00 - 15:20	**BIOINFO-CORE**
11:00 - 15:20	**BOSC**
11:00 - 15:20	**CAMDA**
11:00 - 15:20	**COVID-19**
11:00 - 15:20	**iRNA**
11:00 - 15:20	**MLCSB**
11:00 - 15:20	**Special Session: Single Cell and Spatial Data Analysis**
11:00 - 15:20	**SysMod**
11:00 - 15:20	**Tech Track**
11:00 - 15:20	**VarI**

12:20	Programme Break
12:40	Sessions Continue
14:00	Programme Break
14:20	Sessions Continue
15:20	ISCB Accomplishments by a Senior Scientist Award Keynote: Peer Bork, EMBL Heidelberg Introduced by: Martin Vingron, ISCB Awards Committee Chair
16:20	Closing Ceremonies

Special Sessions

SUNDAY, JULY 25 (11:00 – 12:20; 12:40 – 14:00; 14:20 – 15:20 UTC)

https://www.iscb.org/ismbeccb2021-program/special-sessions

SST01: REPRESENTATION LEARNING IN BIOLOGY

ORGANIZER(S):

Christian Dallago, Technical University of Munich, Germany
Ananthan Nambiar, University of Illinois at Urbana-Champaign, United States
Ali Madani, Salesforce Research, United States
Peter Koo, Cold Spring Harbor Laboratory, United States

11:05 **Kevin Yang**
Protein representation learning: Beyond borrowing from Natural Language Processing and Computer Vision

11:35 **Neil Thomas**
Single Layers of Attention Suffice to Predict Protein Contacts

11:50 **Hideki Yamaguchi**
Evotuning protocols for Transformer-based variant effect prediction on multi-domain proteins

11:55 **Dan Ofer**
ProteinBERT: A universal deep-learning model of protein sequence and function

12:00 **Dionizije Fa**
Graph attention network based representation learning for cancer drug response prediction and interpretation

12:05 **Alex Rives**
Architectures and training procedures

12:40 **Maria Rodriguez Martinez**
AI-driven engineering of the immune system

12:55 **Paulina Anna Szymczak**
HydrAMP: a deep generative model for antimicrobial peptide discovery

13:00 **Surabhi Vasantrao**
Random Walk-based Matrix Factorization of a Multilayer Network for Protein Function Prediction

13:05 **Hannes Axel Stärk**
Light Attention Predicts Protein Location from the Language of Life

13:10 **Egbert Castro**
Guided Generative Protein Design using Regularized Transformers

13:15 **Smita Krishnaswamy**
Geometric and Topological Approaches to Representation Learning in Biomedical Data

13:30 **Bharath Ramsundar**
ChemBERTa: Self-supervised pretraining for molecular property prediction

13:45 **Yana Bromberg**
Short DNA sequence embeddings uncover metagenome function

14:20 **Burkhard Rost**
Decoding language of life written in protein sequences

14:35 **Farhan Damani**
Multimodal data visualization and denoising Efficient Design of Optimized AAV Capsids using Multi-property Machine Learning Models Trained across Cells, Organs and Species

14:40 **Manik Kuchroo**
Multimodal data visualization and denoising with integrated diffusion

14:45 **Jennifer Listgarten**
Autofocused oracles for model-based design

Special Sessions

SUNDAY, JULY 25 (11:00 – 12:20; 12:40 – 14:00; 14:20 – 15:20 UTC)

https://www.iscb.org/ismbeccb2021-program/special-sessions

SST02: COMPUTATIONAL BIOLOGY GOING GREEN

ORGANIZER(S):

Geoff Barton, University of Dundee, United Kingdom
Alex Bateman, EMBL-EBI, United Kingdom
Michael Inouye, University of Cambridge and Baker Institute, United Kingdom

11:00 **Roy Schwartz**
Green AI

11:40 **Loïc Lannelongue**
Green computing made easy

12:40 **Adrian Friday**
The climate impact of ICT

13:20 **General discussion**

Special Sessions

Tuesday, July 27 (11:00 – 12:20; 12:40 – 14:00; 14:20 – 15:20 UTC)

https://www.iscb.org/ismbeccb2021-program/special-sessions

SST03: NEW DEVELOPMENTS IN AI FOR INTEGRATING IMAGING AND GENOMIC DATA

ORGANIZER(S):

Olivier Gevaert, Stanford University, United States
William Hsu, UCLA, United States
Arvind Rao, University of Michigan, United States

11:00	**Olivier Gevaert**	*Intro to special session*
11:10	**William Hsu**	*Intro to Quantitative imaging & radiomics*
11:20	**Philippe Lambin**	*Integrating handcrated radiomics signatures and molecular data: the example of head and neck cancer and glioblastoma*
11:50	**Evis Sala**	*Integrated Radiogenomic for Unravelling Tumour Hreterogeneity and Treatment Monitoring in Ovarian Cancer*
12:40	**Arvind Rao**	*Intro to digital Pathology*
12:50	**Faisal Mahmood**	*Data-efficient and multimodal computational pathology*
13:20	**Lee Cooper**	*Computational pathology*
14:20	**Anant Madabhushi**	*Interpreter of Maladies: Computational Pathology for Precision Medicine*
14:50	**All Speakers**	*Panel discussion with all speakers*

SST04: EMERGING GAIN-OF-FUNCTION MUTATIONS AND THEIR CHARACTERIZATION BY MULTI-OMICS NETWORK BIOLOGY

ORGANIZER(S):

Zeynep Coban-Akdemir, The University of Texas Health Science Center at Houston, United States
Stephen Yi, The University of Texas at Austin, United States

11:00 **Organizer: Stephen Yi,** The University of Texas at Austin, United States

Welcome and Introduction

11:10 **Keynote: Christopher Burge,** MIT, United States

TBD

11:40 **Keynote: Olga Troyanskaya,** Princeton University, United States

From variants to networks - decoding the human genome

12:10 **Kevin Litchfield, University College London, United Kingdom**

Escape from nonsense-mediated decay associates with anti-tumor immunogenicity

12:40 **Keynote: Yi Xing,** University of Pennsylvania, United States

Genetic variation of RNA processing and modification in human tissues

13:10 **Keynote: John Quackenbush,** Harvard University, United States

A Not-Quite Central Dogma: Variants Alter Regulation and Network Structure

13:40 **Invited Talk: Yu (Brandon) Xia,** McGill University, Canada

Using structural systems biology to probe the impact of mutations on protein networks

13:50 **Invited Talk: Claudia Carvalho,** Pacific NW Research Institute, United States

Impact of complex genomic structural variation in MECP2 duplication syndrome

14:20 **Keynote: Trey Ideker,** University of California, San Diego, United States

Building the Mind of Cancer

14:50 **Keynote: Steven Brenner,** University of California, Berkeley, United States

Interpreting newborn genomes: Prediction potential and pitfalls in pervasive personal genomics, and prospects for a Learning Public Health System

Special Sessions

Friday, July 30 (11:00 – 12:20; 12:40 – 14:00; 14:20 – 15:20 UTC)

https://www.iscb.org/ismbeccb2021-program/special-sessions

SST05: SINGLE CELL AND SPATIAL DATA ANALYSIS

ORGANIZER(S):

Malte Luecken, Helmholtz Center Munich, Germany
Shyam Prabhakar, Genome Institute of Singapore
Florian Schmidt, Genome Institute of Singapore
Fabian Theis, Helmholtz Center Munich, Germany
Barbara Treutlein, ETH Zürich, Switzerland

11:00 **Joseph Powell,** Director of the Garvan-Weizmann Centre for Cellular Genomics, Australia

Single-cell eQTL mapping identifies cell type specific genetic control of autoimmune disease

11:30 **Zemin Zhang,** Biomedical Pioneering Innovation Centre Peking University, Beijing, China

Single Cell and Spatial Data Analysis Keynote: Analysis of large-scale single cell transcriptome data for tumor-infiltrating immune cells

12:00 **Daniel Dimitrov,** Heidelberg University, Faculty of Medicine, and Heidelberg University Hospital, Institute for Computational Biomedicine, Germany

Comparison of Resources and Methods to infer Cell-Cell Communication from Single-cell RNA Data

12:05 **Keynote: Bobby Ranjan**, Genome Institute of Singapore, A∗STAR, Singapore

DUBStepR: correlation-based feature selection for clustering single-cell RNA sequencing data

12:10 **Marius Lange,** Helmholtz Zentrum München, Germany

CellRank for directed single-cell fate mapping

12:15 **Wei Vivian Vivian, Rutgers,** The State University of New Jersey, United States

MAAPER: model-based analysis of alternative polyadenylation using 3' end-linked reads

12:40 **Sandhya Prabhakaran,** Moffitt Cancer Center, United States

Sparcle: assigning transcripts to cells in multiplexed images

12:53 **Ruben Dries,** Boston University School of Medicine, United States

Giotto suite, a flexible and high-performing framework for spatial multi-modal analysis

13:06 **Ricardo Omar Ramirez Flores,** Heidelberg University, Faculty of Medicine, and Heidelberg University Hospital, Institute for Computational Biomedicine, Germany

Spatial multi-omic map of human myocardial infarction

13:20 **Shadi Darvish Shafighi,** University of Warsaw, Poland

TUMOROSCOPE: Inferring a map of tumor subclones from Spatial Transcriptomics and bulk DNA sequencing data

13:34 **Yingxin Lin,** The University of Sydney, Australia

scJoint: transfer learning for data integration of atlas-scale single-cell RNA-seq and ATAC-seq

13:47 **Jonas Simon Fleck, ETH Zürich, Switzerland**

Inferring regulomes from multi-modal single-cell measurements with Pando

14:20 **Sarah A. Teichmann,** FMedSci FRS, Cellular Genetics Programme Head, Wellcome Sanger Institute Director of Research, Cavendish Laboratory, Univ. Cambridge

Single Cell and Spatial Data Analysis Keynote: Multi-omic data integration to investigate tissue architecture

14:50 **Samantha A Morris,** Assistant Professor of Developmental Biology and Genetics, Allen Distinguished Investigator, New York Stem Cell Foundation Robertson Investigator, Washington University School of Medicine

Single Cell and Spatial Data Analysis Keynote: New single-cell technologies to dissect reprogramming and development

Birds of a Feather (BoF)

SUNDAY, JULY 25 • WEDNESDAY, JULY 28 • THURSDAY, JULY 29

https://www.iscb.org/ismbeccb2021-program/bof

SUNDAY, JULY 25, 15:20 - 16:20 UTC

INTERPRETABILITY OF MACHINE LEARNING ALGORITHMS

ORGANIZER(S):

Thomas Y. Chen, U.S. Technology Policy Committee

LOCATION: CafeConnect Round Table Group

WEDNESDAY, JULY 28, 15:20 - 16:20 UTC

BIOINFORMATICS ADVANCES: MEET THE EDITORS

ORGANIZER(S):

Thomas Lengauer, Editor-in-Chief; Max Planck Institute for Informatics; University of Cologne

LOCATION: Research Exchange Forum

WEDNESDAY, JULY 28, 15:20 - 16:20 UTC

JBROWSE

ORGANIZER(S):

Scott Cain, Ontario Institute for Cancer Research

LOCATION: Research Exchange Fortum

WEDNESDAY, JULY 28, 15:20 - 16:20 UTC

JALVIEW AND FRIENDS

ORGANIZER(S):

Jim Procter, University of Dundee

LOCATION: Research Exchange Forum

THURSDAY, JULY 29, 15:20 - 16:20 UTC

NEXT STEPS FOR COMPUTATIONAL REPRODUCIBILITY TOWARD FULLY EXECUTABLE PAPERS

ORGANIZER(S):

Geraldine Van der Auwera, Broad Institute

LOCATION: CafeConnect Round Table Group

THURSDAY, JULY 29, 15:20 - 16:20 UTC

INTEROPERABILITY CHALLENGES FOR SENSITIVE BIOMEDICAL DATA

ORGANIZER(S):

Caitlin McHugh, Alzheimer's Disease Data Initiative (ADDI)

LOCATION: Research Exchange Forum

THURSDAY, JULY 29, 15:20 - 16:20 UTC

NEW METHODS OF PROGRAMMATIC, WEB AND CLOUD DATA ACCESS FROM NCBI

ORGANIZER(S):

Nuala O'Leary, NCBI/NLM/NIH

LOCATION: Research Exchange Forum

COVID-19 Special Track

FRIDAY, JULY 30

https://www.iscb.org/cms_addon/conferences/ismbeccb2021/tracks/covid-19

11:00 *COVID-19 Track and Panel*

11:10 ***Tim Hubbard**, Kings College London, United Kingdom*
***Sebastian Mauer-Stroh**, A*STAR, Singapore*
***David Carr, Wellcome Trust**, United Kingdom*
***Tulio de Oliveira**, University of KwaZulu-Natal, South Africa*
***Guy Cochrane,** Director of the Nucleotide Archive, European Bioinformatics Institute, United Kingdom*

COVID-19 Panel: data sharing, access and protection

12:05 ***Martina Kutmon**, Maastricht University, Netherlands*

WikiPathways as a platform for COVID-19 pathway models

12:40 ***Michal Linial**, The Hebrew University of Jerusalem, Israel*

Revealing SARS-CoV-2 protein architectures and function by integrating modeling and in situ MS proteomics

12:55 ***Mahdi Moosa**, University at Buffalo, United States*

Host stress granule hijacking by Coronavirus nucleocapsids: Potential roles of protein intrinsic disorder and liquid-liquid phase separation

13:10 ***Tomer M Yaron**, Weill Cornell Medicine, United States*

The Phosphorylation Model of SARS-CoV-2 Nucleocapsid Protein

13:25 ***Liang Huang**, Baidu Research USA; Oregon State University, United States*

Efficient Algorithms for Optimized mRNA Sequence Design

13:40 ***Gabriela Merino**, SINC-CONICET-FICH-UNL/IIB-UNER, Argentina*

A Machine Learning approach for pre-miRNA discovery in SARS-CoV-2

14:20 ***Jing Xing,** Michigan State University, United States*

Published Anti-SARS-CoV-2 In Vitro Hits Share Common Mechanisms of Action that Synergize with Antivirals

14:35 ***Nicoleta Siminea**, National Institute of Research and Development for Biological Sciences, and University of Bucharest, Romania*

Network controllability analysis for drug repurposing in COVID-19

14:50 ***Nash Rochman**, The National Institutes of Health, United States*

Ongoing Global and Regional Adaptive Evolution of SARS-CoV-2

15:05 ***Omer Noy**, Tel-Aviv University, Israel*
A Machine Learning Model for Predicting Deterioration of COVID-19 Inpatients

POSTERS

SUNDAY, JULY 25 • MONDAY, JULY 26 • TUESDAY, JULY 27 • WEDNESDAY JULY 28 • THURSDAY JULY 29

https://www.iscb.org/cms_addon/conferences/ismbeccb2021/posters.php

Poster Session A:

Sunday, July 25 between 15:20 - 16:20 UTC

3DSIG
Bio-Ontologies
BioVis
HitSeq
SST01: Representation learning in biology
TransMed

Poster Session B:

Monday, July 26 between 15:20 - 16:20 UTC

3DSIG
Bio-Ontologies
BioVis
CompMS
Education
EvolCompGen
HitSeq
NetBio
RegSys
TransMed

Poster Session C:

Tuesday, July 27 between 15:20 - 16:20 UTC

3DSIG
BioVis
CompMS
Education
EvolCompGen
HitSeq
NetBio
RegSys
TransMed

Poster Session D:

Wednesday, July 28 between 15:20 - 16:20 UTC

CAMDA
Education
EvolCompGen
Function
iRNA
MICROBIOME
MLCSB
RegSys
Text Mining

Poster Session E:

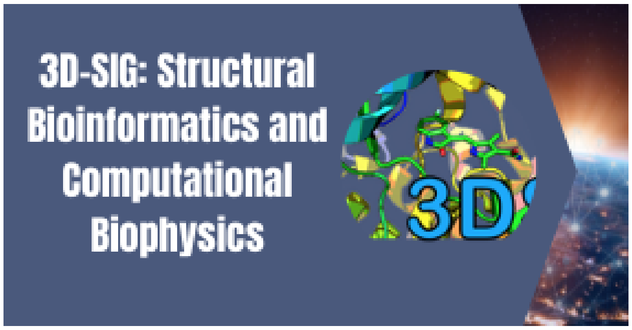
Thursday, July 29 between 15:20 - 16:20 UTC

BIOINFO-CORE
BOSC
CAMDA
COVID-19
EvolCompGen
Function
iRNA
MICROBIOME
MLCSB
RegSys
SST05: Single Cell and Spatial Data Analysis
SysMod
Text Mining
VarI
General Comp Bio

3DSIG COSI

COSI TRACK PRESENTATIONS

SUNDAY, JULY 25TH



11:00 **3DSIG Keynote**
Alex Bateman, EMBL-EBI, United Kingdom
Structure Predictions Transform Protein Family Classification

12:00 **Pawel Szczerbiak,** Malopolska Centre of Biotechnology, Jagiellonian University, Poland
Exploring the microbiome protein structure space using simulations and deep learning

12:40 **Carlos Outeiral Rubiera,** University of Oxford, United Kingdom
How good are protein structure prediction methods at predicting folding pathways?

13:00 **Dea Gogishvili,** Vrije Universiteit Amsterdam, Netherlands
How sticky are your proteins?

13:20 **Sutanu Bhattacharya,** Auburn University, United States
DisCovER: distance- and orientation-based covariational threading for weakly homologous proteins

13:40 **Yuning You,** Texas A&M University, United States
Cross-Modality and Self-Supervised Protein Embedding for Compound-Protein Affinity and Contact Prediction

14:20 **Eddy Elisée,** Génomique Métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, France
MODAMDH: identification of diverse Amine Dehydrogenases by screening biodiversity using sequence and structure-based approaches

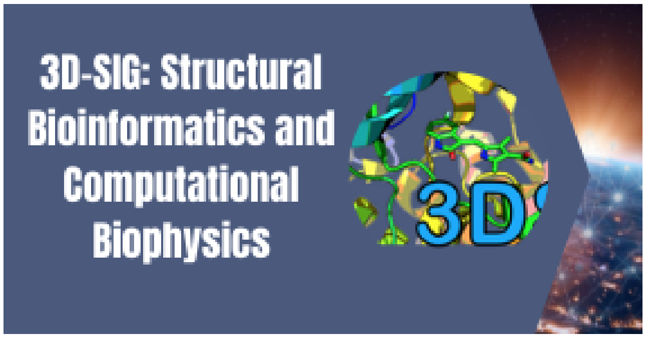
14:40 **Maxim Tsenkov,** University of Dundee, United Kingdom
Exploring human population variation and three-dimensional structures in the Armadillo repeat family

15:00 **Nan Xu,** USC, United States
Graphical Models For Identifying Pore-forming Family Proteins In The Twilight Zone

3DSIG COSI

COSI TRACK PRESENTATIONS

Monday, July 26th

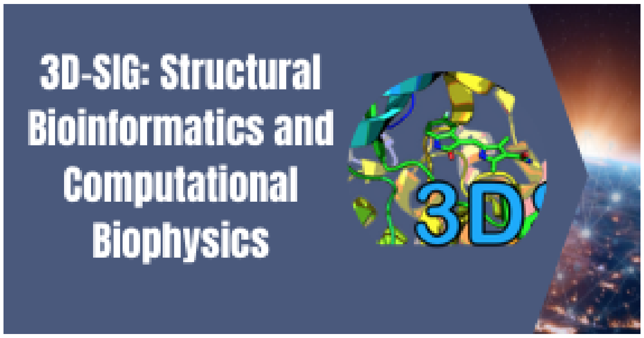


11:00	**Eldad Haber,** Genomica AI, Canada	*Deep Relaxed Complex Scheme*
11:20	**Okke Melse,** TUM Center for Protein Assemblies and TUM School of Life Sciences, Technische Universität München, Germany	*Strategies to Improve the Description of Ligand Binding Sites in Metalloproteins for Biomolecular Simulations.*
11:40	**Jochen Sieg,** Universität Hamburg, Germany	*Data-Driven Analysis of Single Point Mutations through Rapid Scan of 3D Micro-Environments*
12:00	**Martin Schwersensky,** Université Libre de Bruxelles, Belgium	*Large-scale in silico mutagenesis experiments reveal optimization of genetic code and codon usage for protein mutational robustness*
12:40	**Mallika Iyer,** Sanford Burnham Prebys Medical Discovery Institute, United States	*Assessing the conservation of large-scale conformational movements in homologous proteins using a novel metric based on difference distance maps*
13:00	**Markus Schneider,** Technical University of Munich, Germany	*SenseNet: A Cytoscape3-plugin for analysis of MD-based interaction networks*
13:20	**Jacob Piland,** University of Notre Dame, United States	*Dynamic networks improve protein structural classification*
13:40	**Daniel Berenberg,** New York University, United States	*Graph embeddings for protein structural comparison*
14:20	**Zofia Parteka,** Centre of New Technologies, University of Warsaw, S. Banacha 2c, 02-097 Warsaw, Poland, Poland	*Three dimensional computational visualization of a distinct chromatin loop in human lymphoblastoid cells by super resolution imaging*
14:40	**Matic Pavlin,** University of Ljubljana, Faculty of Electrical Engineering, Slovenia	*All-Atom Molecular Simulations of a Type II DNA Topoisomerase Molecular Motor*

3DSIG COSI

COSI TRACK PRESENTATIONS

Tuesday, July 27th



11:00 **Bruna Moreira da Silva,** The University of Melbourne, Australia

Predicting conformational B-cell epitopes using graph-based signatures

11:20 **K. Anton Feenstra,** Vrije Universiteit, Amsterdam, Netherlands

Sequence-based Interface Prediction for Conformational Epitopes

11:40 **Constantin Schneider,** University of Oxford, United Kingdom

DLAB - Deep learning methods for structure-based virtual screening of antibodies

12:00 **Vadim Karnaukhov,** Skoltech, Russia

TCRen: a statistical potential for residue interaction that accurately predicts TCR:peptide recognition

12:40 **Peiyuan Feng,** Institute for Interdisciplinary Information Sciences, Tsinghua University, Beijing, China, China

Proceedings Presentation*: Predicting MHC-peptide binding affinity by differential boundary tree*

13:00 **Alexandre G. De Brevern,** University of Paris, France

Contribution of bioinformatics to blood transfusion: database and 3D intraprotein interaction studies

13:20 **Ayele Abaysew,** Technology and Innovation Institute, Ethiopia

SARS-CoV-2 genome variants epidemiology surveillance in Ethiopia and dynamic mutational change of S Spike protein through computational analysis

13:40 **Michal Linial,** The Hebrew University of Jerusalem, Israel

Revealing SARS-CoV-2 protein architectures through in-situ MS proteomics and integrative modeling

14:20 **R. Gonzalo Parra,** European Molecular Biology Laboratory (EMBL), Heidelberg, Germany, Germany

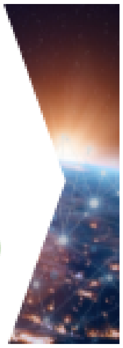
Energetic Local Frustration across NMR Structures in the Protein Data Bank

14:40 **Final Remarks**

BIOINFO-CORE

COSI TRACK PRESENTATIONS

Friday, July 30th



11:00 **Nicole Scherer**
An alien in a hospital data center: solitary management of a bioinformatics platform

11:10 **Gregg TeHennepe**
Accelerating the Velocity of Team Data Science with Research Project Management

11:20 **Fatima Mitterboeck,** Agriculture and Agri-Food Canada, Canada
The Bioinformatics Research Support Network at Agriculture and Agri-Food Canada

11:30 **Fleur Gawehns,** NIOO-KNAW/KWS Vegetables, the Netherlands
Building up a bioinformatics community at the Dutch institute for ecology

11:40 **Krishna Karuturi,** The Jackson Laboratory, United States
Embracing Advances in Machine Learning & Imaging for Biomedical Research

11:50 **Ning Zhang**
RiboSeeker: An End-to-End Package for Ribosome Profiling Data Analysis

12:40 **Johannes Köster,** University of Duisburg-Essen, Germany
***BIOINFO-CORE Keynote**: Reproducible, adaptable, transparent, and composable data analyses with Snakemake*

13:20 *Breakout room setup*

13:30 *Breakout room discussion 1*

14:20 *Breakout room report 1*

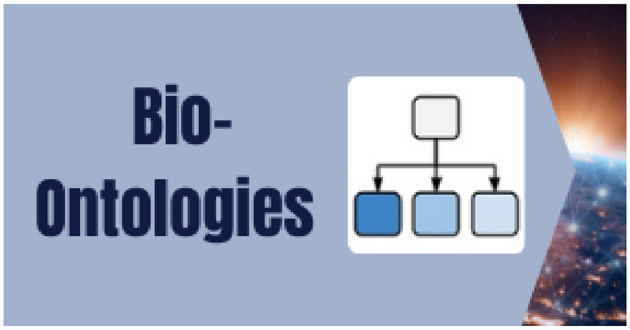
14:30 *Breakout room discussion 2*

15:00 *Breakout room report 2*

Bio-Ontologies COSI

COSI TRACK PRESENTATIONS

Sunday, July 25th



11:00 **Marinka Zitnik,** Harvard Medical School, United States

BIO-ONTOLOGIES COSI KEYNOTE: *Actionable Machine Learning for Drug Discovery and Development*

12:40 **Sanya Taneja,** University of Pittsburgh, United States

Designing potential extensions from G-SRS to ChEBI to identify natural product-drug interactions

13:00 **Jinzhou Yang,** Maastricht University, Institute of Data Science, Netherlands

Publishing Medical Context of Neurological Drug Indications as a Knowledge Graph

13:20 **Sarah Mullin,** Yale University, United States

Chemical Entity Normalization for Successful Translational Development of Alzheimer's Disease and Dementia Therapeutics

13:40 **Jie Zheng,** ShanghaiTech University, China

Proceedings Presentation: KG4SL: Knowledge Graph Neural Network for Synthetic Lethality Prediction in Human Cancers

14:20 **Núria Queralt Rosinach,** Leiden University Medical Center, Netherlands

The COVID-19 epidemiology and monitoring ontology

14:40 **Thomas Joseph,** Tata Consultancy Services Ltd, India

Biomedical Text-Mining for Rare Disease Dictionary Augmentation

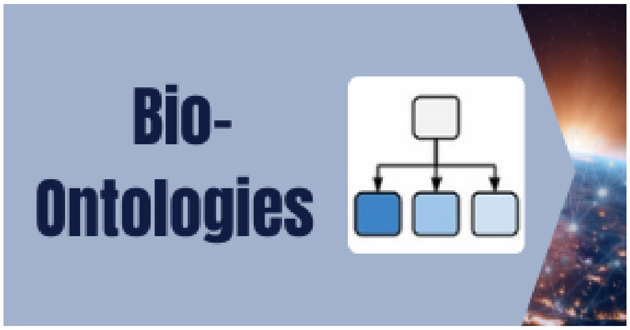
15:00 **Tiago Lubiana,** University of São Paulo, Brazil

Wikidata for 5-star Linked Open Databases: a case study of PanglaoDB

Bio-Ontologies COSI

COSI TRACK PRESENTATIONS

Monday, July 26th



11:00 **Matthias Samwald**

BIO-ONTOLOGIES COSI KEYNOTE: Aligning Human and Machine Intelligence

12:40 **Susana Nunes,** LASIGE, Faculdade de Ciências, Universidade de Lisboa, Portugal

Predicting Gene-Disease Associations with Knowledge Graph Embeddings over Multiple Ontologies

13:00 **Sarah Alghamdi,** King Abdullah University of Science and Technology, Saudi Arabia

How much can model organism phenotypes teach us about human disease? A study using ontologies and semantic machine learning

13:20 **Cen Wan,** Birkbeck, University of London, United Kingdom

Elucidating human ageing-related phenotypic abnormalities with hierarchical feature selection method

13:40 **Bio-Ontologies Community**

Bio-Ontologies COSI Community Plenary

ISCB TOWN HALL

MONDAY, JULY 26

10:00 - 1100 UTC

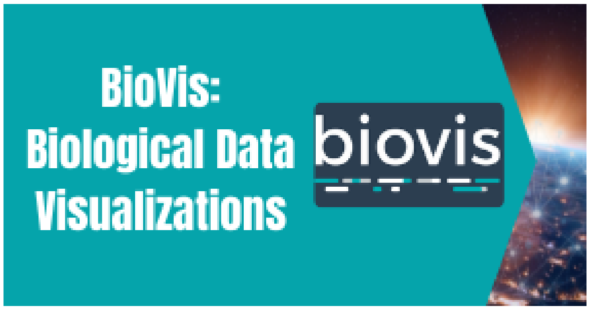
Join us at the ISCB Town Hall meeting to learn more about the latest programs, initiatives, and conferences. This is your chance to help shape the future of ISCB by providing feedback and suggestions.

The Town Hall will close with a celebration of achievement with the announcement of the Wikipedia Competition Award winners, Art in Science Award winners, Student Council Symposium award winners, celebration of the 2021 Class of Fellows, and announcement of the incoming Board of Directors.

BIOVIS COSI

COSI TRACK PRESENTATIONS

Monday, July 26th



11:00 **BioVis Opening**

11:10 **Seán O'Donoghue,** Garvan Institute of Medical Research, Australia

BioVis Keynote: *Inter-disciplinary practices in BioVis*

12:00 **Liz Marai,** University of Illinois at Chicago, United States

BioVis 10th Anniversary - Test of Time Award Ceremony

12:40 **Theresa Anisja Harbig,** Harvard Medical School, United States

Proceedings Presentation: *OncoThreads: Visualization of Large Scale Longitudinal Cancer Molecular Data*

13:00 **Ricardo Humberto Ramirez Gonzalez,** John Innes Centre, United Kingdom

Visualisation of Identical-By-State regions across multiple assembled genomes.

13:10 **Naina Tiwari,** TCS Research, India

Visualization of SARS-CoV-2 Genome Atlas

13:20 **Éloi Durant,** Institut de Recherche pour le Développement, France

A look at trails through the pangenome visualization jungle

13:30 **Sehi L'Yi,** Harvard Medical School, United States

Grammar-Based Interactive Visualization of Genomics Data

13:50 **Theresa Anisja Harbig,** University of Tuebingen, Institute for Bioinformatics and Medical Informatics, Germany

OmicsTIDE: Interactive Exploration of Trends in Multi-Omics Data

14:20 **Qianwen Wang,** Harvard Medical School, United States

State-based Visual Analysis of Disease Progression with ThreadStates

14:40 **Patrick Martin,** BRIC, Denmark

Vesalius: Image-free extraction and analysis of tissue anatomy by using image processing applied to sequencing based Spatial Transcriptomics

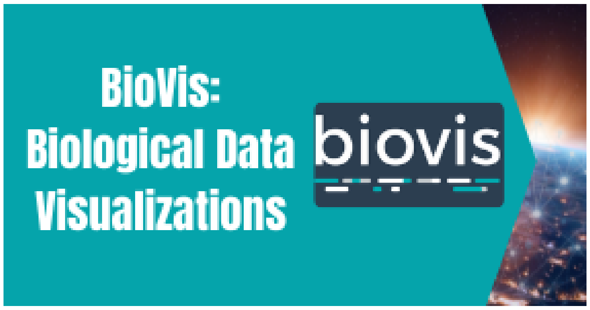
15:00 **Jen Rogers**

BioVis Highlights Talk: Insights From Experiments With Rigor in an EvoBio Design Study

BIOVIS COSI

COSI TRACK PRESENTATIONS

Tuesday, July 27th



11:00 **Komlan Atitey,** NIH - National Institute of Environmental Health Sciences (NIEHS), United States

Benchmarking framework for optimal visualization and interpretability of high-dimensional separable data

11:10 **Qianwen Wang,** Harvard Medical School, United States

Explaining Deep Learning Approaches in Drug Repurposing through Interactive Data Visualization

11:30 **Elzbieta Gralinska,** Max Planck Institute for Molecular Genetics, Germany

Association Plots reveal cluster-specific genes from high-dimensional transcriptome data

11:40 **Mikaela Koutrouli,** University of Copenhagen, Denmark

Color encoding of high-dimensional data using the CIELAB color space and state-of-the-art dimensionality reduction techniques

11:50 **Jayaram Kancherla**, Data Science and Statistical Computing, Genentech, Inc., United States

Hierarchical interactive exploration and analysis of single cell RNA-seq datasets

12:00 **Helena Jambor**

BioVis Highlights Talk: Image visualisation in publications - current status and workflows for improvements

12:40 **Marwan Abdellah,** Blue Brain Project (BBP) / EPFL, Switzerland

Proceedings Presentation: Metaball skinning of synthetic astroglial morphologies into realistic mesh models for in silico simulations and visual analytics

13:00 **Trevor Manz,** Harvard Medical School, United States

Interactive multiscale microscopy visualization on the web with Viv

13:10 **Devin Lange,** University of Utah, United States

Loon: Using Exemplars to Visualize Large Scale Microscopy Data

13:30 **Heba Sailem,** University of Oxford, United Kingdom

ShapoGraphy: a glyph-oriented visualisation approach for creating pictorial representations of bioimaging data

13:50 **Peter Karp,** SRI International, United States

An Extensive Visualization Suite for Pathway/ Genome Databases

14:20 **Jessica Hullman,** Northwestern University, US

BioVis Keynote: *Theories of inference for visualization interactions*

15:10 **BioVis Award Ceremony & Closing**

BOSC COSI

COSI TRACK PRESENTATIONS

Friday, July 30th

BOSC: Bioinformatics Open Source Conference

11:00 **Thomas Hervé Mboa Nkoudou,** University of Ottowa and Mboalab, Canada/Cameroon
BOSC Keynote: Contribution du mouvement maker dans le domaine de la biotechnologie en Afrique: Une perspective de la science ouverte (Contribution of the maker movement to biotechnology in Africa: An open science perspective)

11:40 **Gandham, Pierce-Ward, Herzeel**
Lightning Talks Analysis Tools A

11:40 **Bhanu Gandham,** Broad Institute of MIT and Harvard, United States
GATK for Microbes

11:45 **N. Tessa Pierce-Ward,** University of California, Davis, United States
Sourmash protein k-mer sketches for large-scale sequence comparisons

11:50 **Charlotte Herzeel,** imec, Belgium, Belgium
elPrep 5: A multi-threaded tool for sequence analysis

12:00 **Kunzmann, Twesigomwe, Gatzen**
Lightning Talks Analysis Tools B

12:00 **Patrick Kunzmann,** Technical University Darmstadt, Germany
Novelties in Biotite: A Python library for computational molecular biology

12:05 *StellarPGx: A Nextflow Pipeline for Calling Star Alleles in Cytochrome P450 Genes*

12:10 **Michael Gatzen,** Broad Institute of MIT and Harvard, Germany
Evaluating functional equivalence between variant calling pipelines

12:40 **Kylee Degatano,** Broad Institute, United States
Introducing WARP: A collection of cloud-optimized workflows for biological data processing and reproducible analysis

13:00 **Junjun Zhang,** Ontario Institute for Cancer Research, Canada
WFPM: a novel WorkFlow Package Manager to enable collaborative workflow development via reusable and shareable packages

13:20 **Paolo Di Tommaso,** Seqera Labs, Spain
Evolution of the Nextflow workflow management system

13:40 **Tazro Ohta,** Database Center for Life Science, Japan
Sapporo: an implementation of GA4GH Workflow Execution Service standard to bridge the different workflow language communities

13:50 **Denis Yuen,** Ontario Institute for Cancer Research, Canada
Dockstore - 2021 update

12:00 **Reijnders, Diesh, Cain**
Lightning Talks Visualization

14:20 **Maarten Reijnders,** Department of Ecology and Evolution, University of Lausanne, Switzerland
Summary Visualizations of Gene Ontology Terms With GO-Figure!

14:25 **Colin Diesh,** University of California, Berkeley, United States
JBrowse 2: A data visualization platform with special features for comparative genomics and structural variant visualization

14:30 **Scott Cain,** Ontario Institute for Cancer Research, United States
Using Docker to make JBrowse deployment easier

14:40 **Gemma Turon,** Ersilia Open Source Initiative, United Kingdom
Ersilia: a hub of open source drug discovery models for global health

14:50 **Jeremy Yang,** Indiana University, United States
Knowledge graph analytics platform combining LINCS and IDG for drug target illumination featuring preliminary results for Parkinson's Disease

15:00 **Caralyn Reisle,** Canada's Michael Smith Genome Sciences Centre, Canada
Robust variant interpretation in precision oncology using a graph knowledge base

BOSC COSI

COSI TRACK PRESENTATIONS

Thursday, July 29th

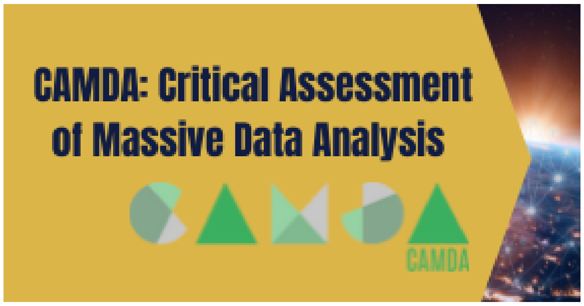
BOSC: Bioinformatics Open Source Conference

11:00	**Harris, Cock, Sponsors,** *Opening remarks*
11:20	**Christie Bahlai,** Kent State University, USA ***BOSC Keynote: Significant heterogeneities: Ecology's emergence as open and synthetic science***
12:00	**Psomopoulos, Deshpande, Selby** *Lightning Talks Standards and Practices for Open Science*
12:00	**Allegra Via,** IBPM-CNR, c/o Department of Biochemical Sciences , Italy *The ELIXIR Software Management Plan*
12:05	**Dhrithi Deshpande,** University of Southern California, United States *Low availability of code and high availability of raw omics data accompanying biomedical studies*
12:10	**Peter Selby,** Cornell University, United States *BrAPI: a standard API specification for plant breeding data*
12:40	**Michael Reich,** University of California San Diego, United States *The GenePattern Notebook Environment*
13:00	**Patil, Campbell, Ramnath** *Lightning Talks Tools for Open Science*
13:00	**Sujay Patil,** Sage Bionetworks, United States *Standardizing biomedical metadata curation using schematic*
13:05	**Jamie Campbell,** The University of Edinburgh, United Kingdom *Cadmus: a pipeline for biomedical full-text retrieval*
13:10	**Risharde Ramnath,** University of Connecticut, United States *Tripal creates online biological, community based web portals for research and analysis*
13:20	**Sarah Zaranek**, Curii Corporation, United States *Building a Federated Data Commons with Arvados*
13:40	**Will Spooner,** Zetta Genomics Ltd., United Kingdom *The OpenCGA genome-optimised data store: accessing a hundred thousand genomes, a billion variants, and a hundred trillion genotypes in real-time.*
14:20	**Iddo Friedberg** *Introduction to joint session with Function COSI*
14:30	**Monique Zahn,** SIB Swiss Institute of Bioinformatics, Switzerland *Completing the functional human proteome together!*
14:40	**Lara Mangravite,** Sage Bionetworks, USA ***BOSC/Function Keynote: Open approaches to advance data-intensive biomedicine***

CAMDA COSI

COSI TRACK PRESENTATIONS

Wednesday, July 28th

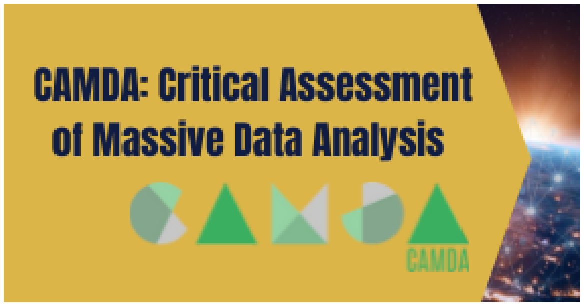


11:00	**Francesca Ciccarelli** ***CAMDA Keynote: Gene deregulations driving cancer at single patient resolution***
12:00	**Wenzhong Xiao,** Massachusetts General Hospital, Harvard Medical School, United States *CAMADA Challenges - Overview*
12:40	**Xianghao Zhan,** Stanford University, United States *Filter Drug-induced Liver Injury (DILI) Literature with Natural Language Processing and Ensemble Learning*
13:20	**Arsentii Ivasiuk,** Bogomoletz Institute of Physiology, Kyiv, Ukraine, Ukraine *Comparative analysis of information-theory-based statistical methods and transformer-based machine learning techniques for text classification*
13:40	**Malik Yousef,** Zefat College, Israel *The CAMDA Contest Challenges TextNetTopics: Applied on Literature AI for Drug Induced Liver Injury*
13:50	**Gehad Youssef,** University of Cambridge, United Kingdom *Medical text classification using dynamic time warping (DTW) and a CNN-BiLSTM hybrid model*
14:20	**Serghei Mangul,** University of Southern California, Los Angeles, United States *Robustness and reproducibility of computational genomics tools*
14:30	**Michał Kowalski,** Krakow, Poland, Poland *In silico evaluation of SARS-CoV-2 primers performance*
14:40	**Kinza Rian,** Sevilla,, Spain *Mechanistic models of COVID-19 disease maps to model SARS-CoV-2 infection and \antiviral interventions*
14:50	**Joaquin Dopazo,** Sevilla, Spain *CAMDA 1st day summary*

CAMDA COSI

COSI TRACK PRESENTATIONS

Thursday, July 29th



11:00 **Weida Tong**
CAMDA Invited: 5 myths about AI and its implication to regulatory science at FDA

11:40 **Sanjay Rathee,** University of Cambridge, United Kingdom
DILIc : An AI based classifier to search for Drug-Induced Liver Injury Literature

12:40 **Nicholas M Katritsis,** University of Cambridge, United Kingdom
dialogí: A text-mining approach for the identification of DILI-related literature with automated concept extraction

13:00 **Valentyn Bezshapkin,** Małopolska Centre of Biotechnology, Poland
Fine-tuning pretrained roBERTa model for optimizing relevant biomedical literature search

13:20 **Dimitar Vassilev,** Sofia University , Bulgaria
Discovering relationship between bacteriophages and antimicrobial resistance

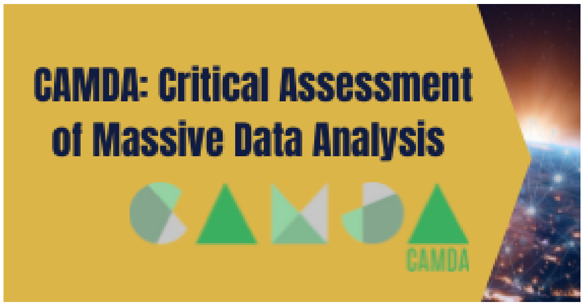
14:20 **Nikos Kyrpides**
CAMDA Keynote: Microbiome Data Science: from the Earth microbiome to the Global virom

15:10 **Paweł P. Łabaj,** Małopolska Centre of Biotechnology of Jagiellonian University, Poland
CAMDA 2nd day summary

CAMDA COSI

COSI TRACK PRESENTATIONS

Friday, July 30th



11:00 **María Peña-Chilet,** Hospital Virgen del Rocío, Sevilla, Spain, Spain

CAMDA Invited: Mechanistic models in emerging infectious diseases: learning from COVID-19

11:40 **Gonghua Li,** Chinese Academy of Sciences, China

Targeting the host response in COVID-19 by integration of metabolic modeling and cheminformatics

12:40 **Dongyuan Wu,** Department of Biostatistics, University of Florida, United States

UTRCOV2: Unraveling T cell responses for long term protection of SARS-COV-2 infection

13:00 **Omid Bazgir,** Texas Tech University, United States

Proceedings Presentation: Investigation of REFINED CNN ensemble learning for anti-cancer drug sensitivity prediction

13:20 **Jung Hun Oh,** Memorial Sloan Kettering Cancer Center, United States

Proceedings Presentation: PathCNN: Interpretable convolutional neural networks for survival prediction and pathway analysis applied to glioblastoma

13:40 **Trevor Frisby,** Carnegie Mellon University, United States

Proceedings Presentation: Asynchronous Parallel Bayesian Optimization for AI-driven Cloud Laboratories

14:20 **Joaquin Dopazo,** Sevilla, Spain, Spain

CAMDA Cafe - Grand challenges of our times

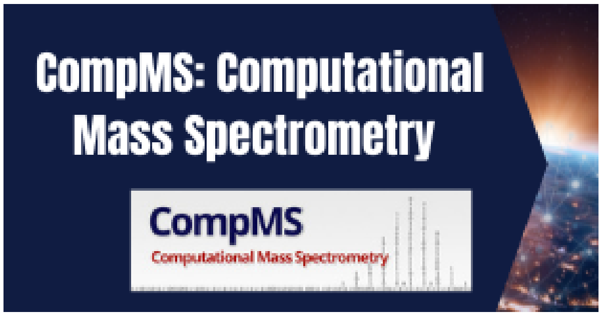
15:10 **David P Kreil**

Award announcement and closing remarks

COMPMS COSI

COSI TRACK PRESENTATIONS

Monday, July 26th



11:00 **Claire O'Donovan**

CompMS Keynote: Developments and challenges in metabolomics and interactions with the other omics

12:00 **Camille Roquencourt,** Gif-sur-Yvette, France, France

ptairMS: processing and analysis of PTR-TOF-MS data for biomarker discovery in exhaled breath

12:40 **Martin Andre Hoffmann,** Friedrich Schiller University Jena, Germany

Assigning confidence to structural annotations from mass spectra with COSMIC

13:00 **Eric Bach,** Aalto University, Finland

Probabilistic Framework for Integration of Mass Spectrum and Retention Time Information in Small Molecule Identification

13:20 **Liu Cao,** Computational Biology Department, Carnegie Mellon University, United States

Proceedings Presentation: MS2Planner: Optimizing Coverage in Tandem Mass Spectrometry based Metabolomics by Iterative Data Acquisition

13:40 **Kyowon Jeong,** University of Tübingen, Germany

FLASHIda: Intelligent data acquisition for top-down proteomics that doubles proteoform identification count

14:20 **Ayse B. Dincer,** University of Washington, United States

Inferring peptide coefficients from quantitative mass spectrometry data

14:40 **Andy Lin, Pacific** Northwest National Laboratory, United States

MS1Connect: a mass spectrometry run similarity measure

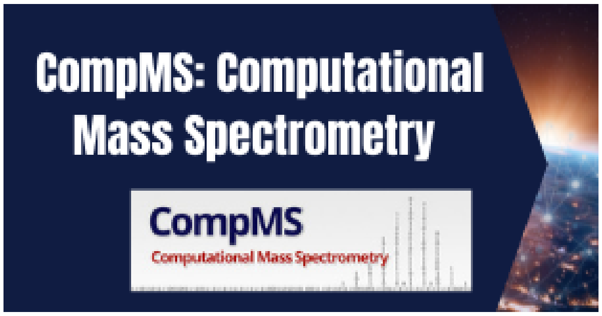
15:00 **Yang Young Lu,** University of Washington, United States

Proceedings Presentation: DIAmeter: Matching peptides to data-independent acquisition mass spectrometry data

COMPMS COSI

COSI TRACK PRESENTATIONS

Tuesday, July 27th



11:00 **Vadim Demichev**

CompMS Keynote: Towards high-throughput proteomics

12:00 **Melanie Föll,** University Medical Center Freiburg, Germany

MaxQuant and MSstats in Galaxy enable reproducible quantitative proteomics in the cloud for everyone

12:10 **Lukasz Kozlowski,** University of Warsaw, Poland

Isoelectric Point Calculator 2.0 - prediction of isoelectric point and pKa dissociation constants

12:40 **Sander Willems,** Max Planck Institute of Biochemistry, Martinsried, Germany, Germany

AlphaTims: Indexing unprocessed trapped ion mobility spectrometry – time of flight data for fast and easy accession and visualization

13:00 **Jinghan Yang, Chinese Academy of Sciences, Beijing, China**

ProteoPeptides: a web-based tool for accurate prediction and visualization of proteotypic peptides in proteomics

13:10 **Charlotte Adams,** University of Antwerp, Belgium

Reprocessing of MS-based virus-host protein interaction data to explore the role of post-translational modifications during SARS-CoV-2 infection

13:20 **Matteo Manica,** IBM Research Europe, Switzerland

Proceedings Presentation: On the Feasibility of Deep Learning Applications Using Raw Mass Spectrometry Data

13:40 **William Fondrie,** University of Washington, United States

Learning compact representations of high-resolution tandem mass spectra without supervision

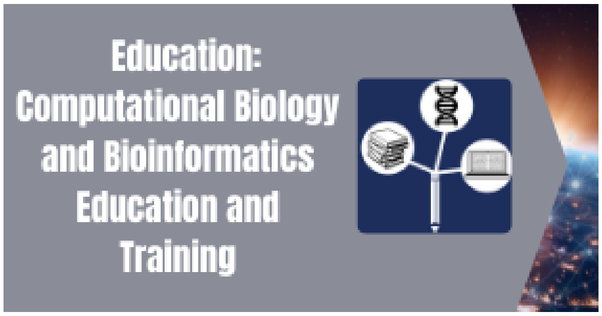
14:20 **Edward Huttlin,** Harvard Medical School, United States

CompMS Keynote: Exploring the 'Social Network' within a Human Cell

EDUCATION COSI

COSI TRACK PRESENTATIONS

Monday, July 26th



11:00 **Allegra Via,** IBPM-CNR, c/o Department of Biochemical Sciences , Italy
EDUCATION COSI KEYNOTE: Teaching the Instagram generation: a lesson learned in the pandemic era

11:40 **Marta Lloret-Llinares,** European Bioinformatics Institute (EMBL-EBI), United Kingdom
The PerMedCoE competency framework to guide the training programme

12:00 **Dr Nikiforos Karamanis,** European Bioinformatics Institute, United Kingdom
User Experience Design training in a bioinformatics organisation

12:40 **Invited Group presentation**
Report from the Bioinformatics Education Summit

12:40 **Invited Group presentation**
Report from the ISCB Education Committee

13:20 **Venkata Satagopam,** University of Luxembourg, Luxembourg
Catherine Brooksbank, EMBL-EBI, United Kingdom
Nicola Mulder, University of Cape Town, South Africa
Report from the ISCB Education Committee

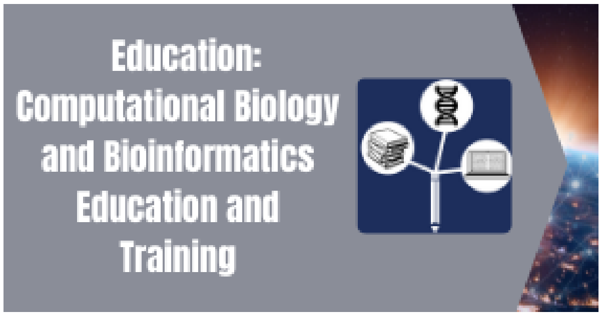
14:20 **Phillip Compeau,** Carnegie Mellon University Computational Biology Department, United States
Teaching a Comprehensive Introductory Course in Computational Biology for First-Year Computer Science Undergraduates

14:40 **Alejandro Reyes Muñoz**
EDUCATION COSI KEYNOTE: Establishing a graduate program in Bioinformatics in Colombia. Challenges and successes from Uniandes experience

EDUCATION COSI

COSI TRACK PRESENTATIONS

Tuesday, July 27th



11:00 **Wai Keat Yam,** Perdana University, Malaysia

EDUCATION COSI KEYNOTE: Journey into Bioinformatics and Data Science Education, Training and Outreach: Our Experience.

11:40 **Bruno Gaeta,** UNSW Sydney, Australia

Assessing understanding of simple bioinformatics algorithms with the Moodle quiz "formulas" question type

12:00 **Marie Semon,** ENS de Lyon / LBMC, France

Practicals in next-generation sequencing - Programming course in a generalist school can truly be fun, even in lockdown.

12:40 **Anna Swan,** EMBL-EBI, United Kingdom

Redesign and FAIRification of EMBL-EBI's training website

13:00 **Pramesh Singh,** Reed College, United States

Graphery: interactive tutorials for biological network algorithms

13:20 **Verena Ras,** University of Cape Town, South Africa

Training during a pandemic: "Why moving online is not the quick fix you think it is" - the H3ABioNet experience

13:40 **Sanna Abrahamsson,** Gothenburg University, Sweden

Proceedings Presentation: Comparison of online learning designs during the COVID-19 pandemic within Bioinformatics courses in higher education

14:20 **Phillip Compeau,** Carnegie Mellon University Computational Biology Department, United States
Vera Matser, European Molecular Biology Laboratory - European Bioinformatics Institute (EMBL-EBI) & ELIXIR-EBI, United Kingdom
Bruno Gaeta, UNSW Sydney, Australia
Nicola Mulder, University of Cape Town, South Africa

Panel Discussion: Online and hybrid education post-COVID

EVOLCOMPGEN COSI

COSI TRACK PRESENTATIONS

MONDAY, JULY 26TH

EvolCompGen: Evolution & Comparative Genomics

EvolCompGen

11:00	**Salvatore Cosentino,** The University of Tokyo, Japan *SonicParanoid2: Machine Learning-Driven Integration of BBH and Protein Domain Analysis for Faster and More Accurate Orthology Inference*
11:40	**Inhyuk Song,** Pusan National University, South Korea *Convolutional neural networks for copy number variation detection in cancer genomes using short-read sequencing data only*
12:00	**Sophie Seidel,** ETH Zurich, Switzerland *Inferring single-cell trees alongside cell-state transition dynamics from lineage tracing and RNAseq data - revised*
12:10	*Live Q&A*
12:40	**Qiqing Tao,** Temple University, United States *Proceedings Presentation: Data-driven speciation tree prior for better species divergence times in calibration-poor molecular phylogenies*
13:10	**Yuval Tabach,** The Hebrew University-Hadassah Medical School, Israel *Co-evolution based machine-learning for predicting human functional interactions and unraveling evolutionary insights*
13:30	**Chris Papadopoulos,** Institute for Integrative Biology of the Cell (Université Paris-Saclay, CEA, CNRS), France *Intergenic ORFs as elementary structural modules of de novo gene birth and protein evolution*
13:50	*Live Q&A*
14:20	**Erin Molloy,** University at California, Los Angeles, United States *Proceedings Presentation: Advancing admixture graph estimation via maximum likelihood network orientation*
14:50	**Yi-Fei Huang,** Pennsylvania State University, United States *Dissecting genomic determinants of positive selection with an evolution-guided regression model*
15:10	*Live Q&A*

EVOLCOMPGEN COSI

COSI TRACK PRESENTATIONS

TUESDAY, JULY 27TH

EvolCompGen: Evolution & Comparative Genomics

EvolCompGen

11:00	**Janani Ravi,** Michigan State University, USA, United States *MolEvolvR: A webapp for characterizing proteins using molecular evolution and phylogeny*
11:40	**Mohak Sharda,** National Centre for Biological Sciences, Bangalore, India, India *Evolutionary and Comparative genomics of Bacterial Non-homologous End Joining Repair*
12:00	**Ilana Brito,** Cornell University, United States *Near-perfect predictions of horizontal gene transfer and the emergence of antibiotic resistance*
12:10	*Live Q&A*
12:40	**Yoann Anselmetti,** Université de Sherbrooke, Canada *Proceedings Presentation: Gene Tree and Species Tree Reconciliation with Endosymbiotic Gene Transfer*
13:10	**Magda Markowska,** University of Warsaw, Poland *CONET: Copy number event tree model of evolutionary tumor history for single-cell data*
13:30	**Conor Walker,** EMBL - European Bioinformatics Institute, United Kingdom *Accurate detection of interspecific positive selection using convolutional neural networks*
13:50	*Live Q&A*
14:20	**Chaitanya Aluru,** Princeton University, United States *Proceedings Presentation: Improved Inference of Tandem Domain Duplications*
14:50	**Malay Basu,** University of Alabama, Birmingham, United States *Linguistic modeling of proteome complexity in cancer: evolutionary Implications*
15:10	*Live Q&A*

EVOLCOMPGEN COSI

COSI TRACK PRESENTATIONS

WEDNESDAY, JULY 28TH

EvolCompGen: Evolution & Comparative Genomics

EvolCompGen

11:00 **Elise Parey,** Institut de Biologie de l'Ecole normale supérieure (IBENS), France
Combining synteny and sequence-based approaches to investigate genome evolution after polyploidization

11:40 **Bastian Pfeifer,** Institute for Medical Informatics, Statistics and Documentation. Medical University Graz, Austria
Detection and quantification of introgression using Bayesian inference based on conjugate priors

12:00 **Dana Sherill-Rofe,** Hebrew University, Israel
Identifying novel biological pathways through phylogenetic profiling based network analysis

12:40 **Kevin Liu,** Michigan State University, United States
Proceedings Presentation: Build a Better Bootstrap and the RAWR Shall Beat a Random Path to Your Door: Phylogenetic Support Estimation Revisited

13:10 **Senbai Kang,** University of Warsaw, Poland

SIEVE: Joint Inference of Tumor Phylogeny and Variant Calling from Single-cell DNA Sequencing Data

13:30 **Elysia Saputra,** University of Pittsburgh, United States
phyloConverge: a likelihood-based approach to identify genomic regions underlying phenotypic convergence at nucleotide resolution

13:50 *Live Q&A*

14:20 **Mattéo Delabre,** University of Montreal, Canada
Super-Reconciliation with Horizontal Gene Transfers

14:40 **Louxin Zhang**
Nadia El-Mabrouk, Université de Montréal, Canada
Dannie Durand, Carnegie Mellon University, United States

EvolCompGen panel discussion

FUNCTION COSI

COSI TRACK PRESENTATIONS

WEDNESDAY, JULY 28TH

11:00 **Ronghui You,** Fudan University, China

Proceedings Presentation: DeepGraphGO: graph neural network for large-scale, multispecies protein function prediction

11:20 **Davide Baldazzi,** University of Bologna - Biocomputing Group, Italy

BENZ WS annotates sequences of the human reference proteome with four level EC numbers

11:40 **Jordan Sicherman,** Graduate Program in Bioinformatics, Canada

Large-scale mining of differential expression data reveals insight into gene function

12:00 **Qinkai Wu,** Graduate Program in Bioinformatics, University of British Columbia, Canada

Cellular composition variation drives coexpression-based gene function prediction

12:40 **Damiano Piovesan,** University of Padova, Italy

Critical assessment of protein intrinsic disorder prediction

13:00 **Jeffrey Yunes,** Yunes Foundation for Research on Aging, Portsmouth, NH, USA, United States

Proposals to improve CAFA evaluation based on community participation

13:20 **Predrag Radivojac, Iddo Friedberg, Mark Wass**

Panel Discussion of CAFA

14:20 **Katharina Waury,** Vrije Universiteit Amsterdam, Netherlands

Sequence-based prediction of proteins associated with extracellular vesicles

14:40 **Sandra Orchard** EMBL-EBI

UniProt and Gene Ontology: the need for functional annotation across the span of taxonomic biodiversity

FUNCTION COSI

COSI TRACK PRESENTATIONS

THURSDAY, JULY 29TH

11:00 **Rıza Özçelik, Boğaziçi University, Turkey**

ChemBoost: A chemical language based approach for the prediction of protein - ligand binding affinity

11:20 **Rıza Özçelik,** Boğaziçi University, Turkey

Ensemble learning for novel drug - target affinity prediction

11:40 **Yue Cao,** Texas A&M University, United States

Transformer-based Protein Function Annotation with Joint Sequence-Label Embedding

12:00 **Gabriela Merino,** IBB-CONICET-UNER, Argentina

Integrating multiple information sources for protein function prediction with end-to-end deep learning

12:40 **Meet Barot,** Center for Data Science, New York University, United States

seqSCAN: Unsupervised Classification of Proteins for New Function Discovery.

13:00 **Dustin Hancks,** UT Southwestern Medical Center, United States

Discovery of cellular gene functions using viral genomes

13:20 **Yanbin Yin,** University of Nebraska - Lincoln, United States

dbCAN-PUL: a database of experimentally characterized CAZyme gene clusters and their substrates

14:20 **Iddo Friedberg**

Introduction to BOSC/Function joint session

14:30 **Monique Zahn,** SIB Swiss Institute of Bioinformatics, Switzerland

Completing the functional human proteome together!

14:40 **Lara Mangravite,** Sage Bionetworks, USA

BOSC/Function Keynote: Open approaches to advance data-intensive biomedicine

GENERAL COMP BIO

COSI TRACK PRESENTATIONS

THURSDAY, JULY 29TH

11:00 **Lauren Spirko-Burns,** Temple University, United States
Unifed Methods for Feature Selection in Large-Scale Genomic Studies with Censored Survival Outcomes

11:20 **Huiwen Zheng,** The University of Queensland, Australia
Revealing cell-to-cell variability changes in the aging immune cells by applying accurate gene expression variability metric

11:40 **Atefeh Taherian Fard,** University of Queensland, Australia
Unlocking insights into cellular senescence through single cell transcriptomics of ageing mesenchymal stem cells

12:00 **Pelin Gundogdu,** Progreso y Salud (FPS), Spain
Pathway-primed explainable neural network for scRNA-Seq data

12:40 **Juexin Wang,** University of Missouri, United States
scGNN: a novel graph neural network framework for single-cell RNA-Seq analyses

13:00 **Florian Jeanneret,** Université Paris-Saclay, France
Towards an integrative multi-omics workflow

13:20 **Elan Ness-Cohn,** Northwestern University, United States
Topological Strategies for the Analysis of Rhythmic Dynamics in Transcriptomic Time-Series Data

13:40 **Felix Drost,** Helmholtz Zentrum München, Technische Universität München, Germany
Predicting T Cell Activation for Mutational Epitopes

14:20 **Muhammet Celik,** Bezmialem Vakif University, Istanbul, Turkey
MoSwA: Protein Sequence Diversity Motif Switch Analyser for Viruses

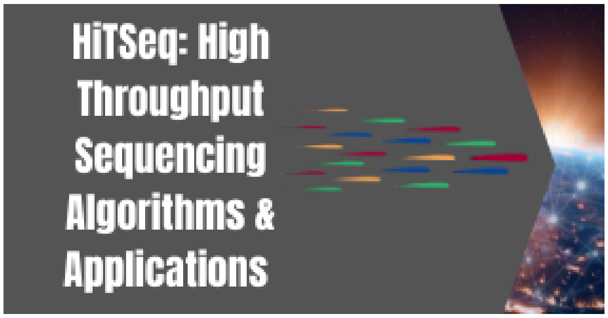
14:40 **David Medina, University of Chile, Chile**
Design of protein variants with desirable properties using Deep Mutational Scanning and Machine Learning approaches

15:00 **Wei Wang,** University of California, Los Angeles, United States
Enhancing Protein-Protein Interaction Prediction with Deep Learning

HITSeq COSI

TRACK PRESENTATIONS

SUNDAY, JULY 25TH



11:00 **Lukas Weilguny,** European Molecular Biology Laboratory, European Bioinformatics Institute, United Kingdom

Dynamic Adaptive Sampling During Nanopore Sequencing and Assembly using Bayesian Experimental Design

11:20 **Mikhail Karasikov,** ETH Zurich, Switzerland

Proceedings Presentation: Topology-based Sparsification of Graph Annotations

11:40 **Jamshed Khan,** University of Maryland, United States

Proceedings Presentation: Cuttlefish: Fast, parallel, and low-memory compaction of de Bruijn graphs from large-scale genome collections

12:00 **Yutong Qiu,** Carnegie Mellon University, United States

Proceedings Presentation: Constructing small genome graphs via string compression

12:40 **Olga Kunyavskaya,** Center for Algorithmic Biotechnology, Saint Petersburg State University, Russia

Proceedings Presentation: CentromereArchitect: inference and analysis of the architecture of centromeres

13:00 **Paul Medvedev,** The Pennsylvania State University, United States

The statistics of \kmers from a sequence undergoing a simple mutation process without spurious matches

13:20 **Sapir Margalit,** Tel Aviv University, Israel

Proceedings Presentation: Long Reads Capture Simultaneous Enhancer-Promoter Methylation Status for Cell-type Deconvolution

13:40 **Laura Tung,** Carnegie Mellon University, United States

Proceedings Presentation: Practical selection of representative sets of RNA-seq samples using a hierarchical approach

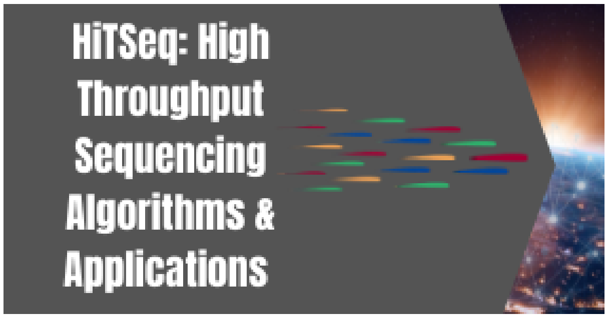
14:20 **Angela Brooks**

HiTSeq Keynote: TBA

HITSeq COSI

TRACK PRESENTATIONS

MONDAY, JULY 26TH



11:00 **Bjarni Halldórsson**

HiTSeq Keynote: TBA

12:00 **Daniel Gibney,** University of Central Florida, United States

Co-linear chaining with overlaps and gap costs

12:40 **Hongyu Zheng,** Carnegie Mellon University, United States

Proceedings Presentation: Sequence-specific minimizers via polar sets

13:00 **Haowen Zhang, Georgia Institute of Technology, United States**

Proceedings Presentation: Real-time mapping of nanopore raw signals

13:20 **Kristoffer Sahlin,** Stockholm University, Sweden

Strobemers: an alternative to k-mers for sequence comparison

13:40 **Richard Lüpken,** Berlin Institute of Health, Germany

Efficient linked-read barcode mapping without read alignment

14:20 **Leah Weber,** University of Illinois at Urbana-Champaign, United States

Proceedings Presentation: doubletD: Detecting doublets in single-cell DNA sequencing data

14:40 **Yang Lu,** University of Washington, United States

ACE: Explaining single-cell cluster from an adversarial perspective

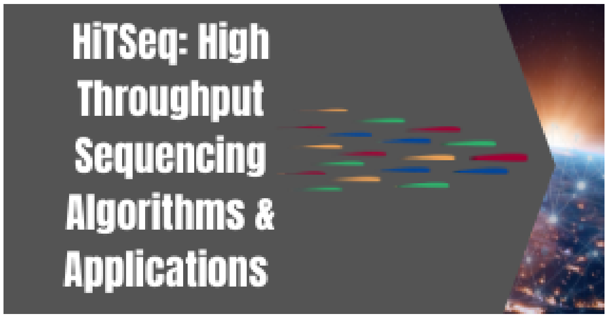
15:00 **Yingxin Cao,** University of California, Irvine, United States

Proceedings Presentation: SAILER: Scalable and Accurate Invariant Representation Learning for Single-cell ATACseq Processing and Integration

HITSeq COSI

TRACK PRESENTATIONS

TUESDAY, JULY 27TH



11:00 **Luca Denti,** Institut Pasteur, France

Comparative genome analysis using sample-specific string detection in accurate long reads

11:20 **Furkan Ozden,** Bilkent University, Turkey

Polishing Copy Number Variant Calls on Exome Sequencing Data via Deep Learning

11:40 **Timofey Prodanov,** University of California San Diego, United States

Robust and accurate estimation of paralog-specific copy number for duplicated genes using whole-genome sequencing

12:00 **Xiao Luo,** Bielefeld University, Germany

phasebook: haplotype-aware de novo assembly of diploid genomes from long reads

12:40 **Xiongbin Kang,** Bielefeld University, Germany

Strainline: full-length de novo viral haplotype reconstruction from noisy long reads

13:00 **Anton Korobeynikov,** Saint Petersburg State University, Russia

BinSPreader: refine binning results for fuller MAG reconstruction

13:20 **Diyue Bu,** Indiana University Bloomington, United States

Proceedings Presentation: Haplotype-based membership inference from summary genomic data

13:40 **Zhiqiang Hu,** University of California, Berkeley, United States

Biological discovery and consumer genomics databases activate latent privacy risk in functional genomics data

14:20 **Steven Salzberg**

HiTSeq Keynote: TBA

MICROBIOME COSI

TRACK PRESENTATIONS

WEDNESDAY, JULY 28TH

11:00	**Shion Hosoda,** Waseda University, Japan *Proceedings Presentation: Umibato: estimation of time-varying microbial interaction using continuous-time regression hidden Markov model*
11:20	**Beatriz García-Jiménez,** Biome Makers Inc., United States *Network properties of fungal soil microbiomes reveal farming practices in vineyard*
11:35	**Vidushi Walia,** TCS Research, India *MAGE: Strain Level Profiling of Metagenome Samples*
11:50	**Aitor Blanco-Miguez,** University of Trento, Italy *Extending and improving metagenomic taxonomic profiling with uncharacterized species*
12:05	**Milot Mirdita,** Max Planck Institute for Biophysical Chemistry, Germany *Fast and sensitive taxonomic assignment to metagenomic contigs*
12:40	**Alice McHardy** *Critical Assessment of Metagenome Interpretation - the second round of challenges*
13:00	**Mihai Pop** *Embracing ambiguity when characterizing microbes*
13:20	**Thilo Muth** *Benchmarking the current state of metaproteomics: a community-driven evaluation of experimental and computational techniques*
13:40	**Wei Wei** *Using the UniFrac metric on whole genome shotgun data*
13:50	**Alexander Sczyrba** *Future CAMI challenges*
14:20	**Yuzhen Ye** ***Microbiome Keynote: Computational methods for mining microbiome multi-omics data***
15:00	**Yancong Zhang,** Harvard T. H. Chan School of Public Health, United States *Proceedings Presentation: Statistical approaches for differential expression analysis in metatranscriptomics*

MICROBIOME COSI

TRACK PRESENTATIONS

THURSDAY, JULY 29TH

11:20 **Jiayu Shang,** City Univeristy of Hong Kong, Hong Kong

Proceedings Presentation: Bacteriophage classification for assembled contigs using Graph Convolutional Network

11:40 **Ruoshi Zhang,** Max Planck Institute for Biophysical Chemistry, Germany

SpacePHARER: sensitive identification of phages from CRISPR spacers in prokaryotic hosts

11:55 **Kangjin Kim,** School of Public Health, Seoul National University, Korea, South Korea

Role of unclassified Lachnospiraceae in the pathogenesis of type 2 diabetes: A longitudinal study of the urine microbiome and metabolites

12:40 **Eran Segal**

Microbiome Keynote: Personalized medicine based on microbiome and clinical data

13:20 **Sofia Forslund**

Fasting alters the gut microbiome reducing blood pressure and body weight in metabolic syndrome patients

13:40 **Giulia Agostinetto,** University of Milano-Bicocca, Italy

SKIOME project: lead skin microbiome research towards data-driven approaches

14:20 **David Pellow,** Tel Aviv University, Israel

SCAPP: An algorithm for improved plasmid assembly in metagenomes

14:35 **Peter Karp,** SRI International, United States

Analyzing Microbial Communities in the Pathway Tools Software

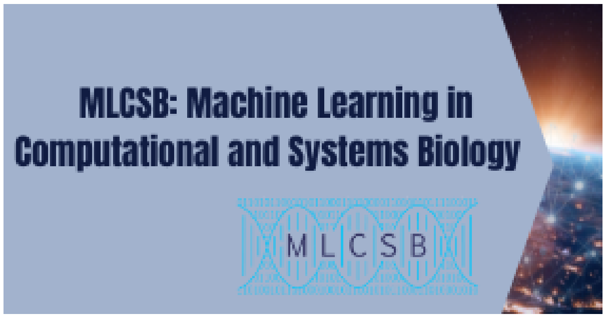
14:50 **Donovan Parks**

Species definitions and the delineation of species in the Genome Taxonomy Database

MLCSB COSI

TRACK PRESENTATIONS

WEDNESDAY, JULY 28TH



11:00 **Ziyang Wei,** University of Chicago, United States

Proceedings Presentation: CALLR: a semi-supervised cell type annotation method for single-cell RNA sequencing data

11:20 **Alexandrina Pancheva,** University of Glasgow, United Kingdom

Using topic modeling to detect cellular crosstalk in scRNA-seq

11:30 **Chen Qiao,** The University of Hong Kong, Hong Kong

Representation learning of RNA velocity reveals robust cell transitions

11:40 **Mohammad Lotfollahi,** Helmholtz Zentrum München, Germany

Learning large-scale perturbation effects in single cell genomics

11:50 **Rohit Singh,** Massachusetts Institute of Technology, United States

Schema: metric learning enables interpretable synthesis of heterogeneous single-cell modalities

12:00 **Shengquan Chen,** Tsinghua University, China

Proceedings Presentation: stPlus: a reference-based method for the accurate enhancement of spatial transcriptomics

12:40 **Alexander P. Wu,** Massachusetts Institute of Technology, United States

Proceedings Presentation: Bayesian information sharing enhances detection of regulatory associations in rare cell types

13:00 **Amirreza Shaeiri,** EMBL-Heidelberg, Iran

Gene Network Connectivity Conveys Robustness in Gene Expression across Individuals, Cell types and Species

13:20 **Adrian L. Sanborn,** Stanford University, United States

Prediction and mechanistic dissection of transcriptional activation protein domains using deep learning and high-throughput screening

13:40 **Julien Martinelli,** Inria/Inserm/Institut Curie, France

Proceedings Presentation: Model learning to identify systemic regulators ofthe peripheral circadian clock

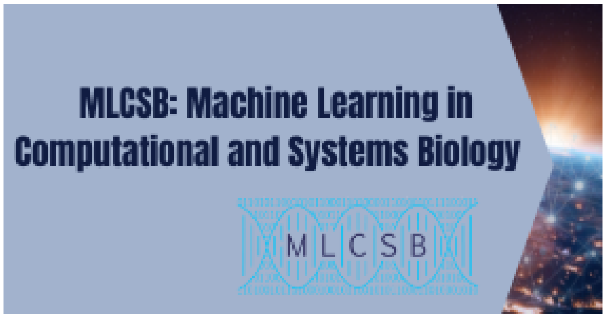
14:20 **Dana Pe'Er,** Memorial Sloan Kettering Cancer Center, United States

MLCSB Keynote: TBC

MLCSB COSI

TRACK PRESENTATIONS

THURSDAY, JULY 29TH



11:00 **Ilayda Beyreli,** Bilkent University, Turkey

Deep multitask learning of gene risk for comorbid neurodevelopmental disorders

11:20 **Asma Nouira,** MINES PARISTECH - Institut Curie - INSERM, France

Multitask group Lasso for Genome-Wide Association Studies in admixed populations

11:40 **Jacob Schreiber,** Stanford University, United States

Navigating the pitfalls of applying machine learning in genomics

12:00 **Yan Cui,** University of Tennessee Health Science Center, United States

Genomic data inequality and multi-ethnic machine learning

12:40 **Emma Pierson**

MLCSB Keynote: Using machine learning to increase health equality

13:20 **Emma Pierson, James Zou, Genevieve Wojcik, Ulrich Hemel**

MLCSB Panel discussion

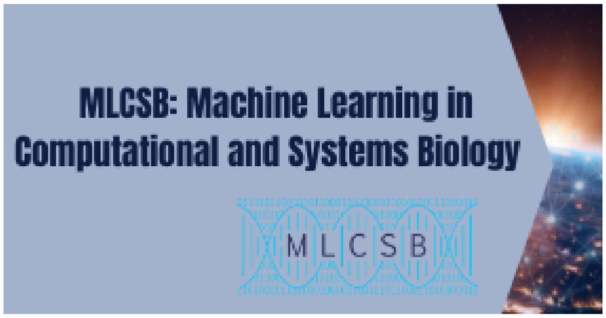
14:20 **Bryan Bryson**

MLCSB Keynote: Algorithms for Infectious Disease

MLCSB COSI

TRACK PRESENTATIONS

FRIDAY, JULY 30TH



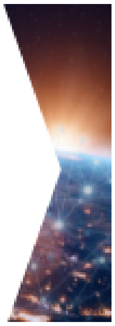
11:00	**Jordi Abante,** Johns Hopkins University, United States *On the estimation of epigenetic energy landscapes from nanopore sequencing data*
11:10	**Thibaud Godon,** Laval University, Canada *RandomSCM: interpretable ensembles of sparse classifiers tailored for omics data*
11:20	**Victoria Li,** Hunter College High School, United States *Proceedings Presentation: CROTON: An Automated and Variant-Aware Deep Learning Framework for Predicting CRISPR/Cas9 Editing Outcomes*
11:40	**Anna Weber,** IBM, Zurich Research Laboratory and ETH Zurich, Switzerland *Proceedings Presentation: TITAN: T Cell Receptor Specificity Prediction with Bimodal Attention Networks*
12:00	**Hannes Stärk,** Department of Informatics, Technical University of Munich, Germany *Light Attention Predicts Protein Location from the Language of Life*
12:40	**Giulio Caravagna,** The Institute of Cancer Research and The University of Trieste, United Kingdom *Subclonal reconstruction of tumors by using machine learning and population genetics*
12:50	**Rafael Peres da Silva,** School of Computing, National University of Singapore, Singapore *Proceedings Presentation: TUGDA: Task uncertainty guided domain adaptation for robust generalization of cancer drug response prediction from in vitro to in vivo settings*
13:10	**Gwanghoon Jang,** Korea University, South Korea *Proceedings Presentation: Predicting mechanism of action of novel compounds using compound structure and transcriptomic signature co-embedding*
13:30	**Tianduanyi Wang,** Aalto University; University of Helsinki, Finland *Proceedings Presentation: Modeling drug combination effects via latent tensor reconstruction*
13:50	**Halil İbrahim Kuru,** Bilkent Universtiy, Turkey *MatchMaker: A Deep Learning Framework for Drug Synergy Prediction*
14:20	**Oznur Tastan,** Sabanci University, Turkey *MLCSB Keynote: Exploiting Molecular Interactions in Machine Learning Models for Cancer*

NETBIO COSI

TRACK PRESENTATIONS

MONDAY, JULY 26TH

NetBio:
Network Biology



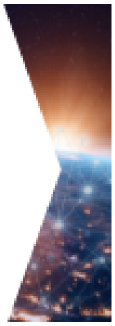
11:00	**Karsten Borgwardt,** ETH Zürich, Switzerland ***NetBio Keynote: Machine Learning Frontiers in Network Biology***
11:40	**Hung-Cuong Trinh,** Ton Duc Thang University, Viet Nam *Proceedings Presentation: A novel constrained genetic algorithm-based Boolean network inference method from steady-state gene expression data*
12:00	**Zakaria Louadi,** Computational Systems Biology, Hamburg University, Germany *Beyond protein-protein interaction networks: Exploring the impact of alternative splicing using DIGGER and NEASE*
12:40	**Victor Popescu,** Åbo Akademi University, Finland *NetControl4BioMed: A web-based platform for controllability analysis of protein-protein interaction networks*
13:00	**Olga Lazareva,** Technical University of Munich, Germany *On the limits of active module identification*
13:20	**James Shiniti Nagai,** RWTH Aachen University Medical School, Germany, Germany *Dissecting differential Cell Cell Communication with CrossTalkeR*
13:40	**Hagai Levi,** Tel Aviv University, Israel *Reducing false GO term calls in network-based active module identification: methodology and a new algorithm*
14:20	**Shawn Gu,** University of Notre Dame, United States *Modeling multi-scale -omics data via a network of networks*
14:40	**Sushmita Roy,** University of Wisconsin-Madison, United States ***NetBio Keynote: Learning Gene Regulatory Networks from Bulk and Single Cell Omic Data***

NETBIO COSI

TRACK PRESENTATIONS

NetBio:
Network Biology

NetBio



TUESDAY, JULY 27TH

11:00 **Jörg Menche**

NetBio Keynote: Network Medicine— From Protein-Protein to Human-Machine Interactions

11:40 **Tunca Dogan,** Hacettepe University, Turkey

CROssBAR: Comprehensive Resource of Biomedical Relations with Knowledge Graph Representations

12:00 **Nikolai Nøjgaard,** IMADA, University of Southern Denmark, Denmark

Proceedings Presentation: Graph Transformation for Enzymatic Mechanisms

12:40 **Juan Shu,** Department of Statistics, Purdue University, United States

Proceedings Presentation: Disease Gene Prediction with Privileged Information and Heteroscedastic Dropout

13:00 **Markus Hoffmann,** Chair of Experimental Bioinformatics, Technical University of Munich, Germany

Simulation, modeling, and network-guided detection of epistasis

13:20 **Louise de Schaetzen van Brienen,** Ghent University, Belgium

GoNetic: Network-Based Driver Identification using Probabilistic Pathfinding

13:40 **Yu Xia,** McGill University, Canada

Mutation Edgotype Drives Fitness Effect in Human

14:20 **Shilu Zhang,** University of Wisconsin-Madison, United States

Inference of cell type-specific gene regulatory networks from single-cell omic datasets

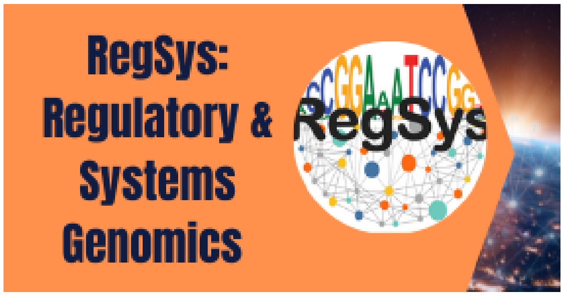
14:40 **Marinka Zitnik,** Harvard Medical School, United States

NetBio Keynote: Few-Shot Learning for Network Biology

REGSYS COSI

TRACK PRESENTATIONS

MONDAY, JULY 26TH



11:00 **Céline Vallot**

COSI REGSYS KEYNOTE: Evolution of epigenomes towards drug resistance in breast cancer

11:40 **Katharina T. Schmid,** Institute of Computational Biology, Helmholtz Zentrum München, Germany

Design and power analysis for multi-sample single cell transcriptomics experiments

12:00 **Anna Hendrika Cornelia Vlot,** Berlin Institute for Medical Systems Biology, Germany

Single-cEll Marker IdentificaTiON by Enrichment Scoring

12:40 **Fabian Theis**

COSI REGSYS KEYNOTE: Learning large-scale perturbation effects in single cell genomics

13:20 **Chao Gao,** University of Michigan, Ann Arbor, MI, USA., United States

Iterative single-cell multi-omic integration using online learning

13:40 **Surag Nair,** Stanford University, United States

Motif syntax determinants of single-cell chromatin dynamics in human somatic cell reprogramming

14:20 **Ieva Rauluseviciute, Norway**

Identification of transcription factor co-binding partners using non-negative matrix factorization

14:40 **Anushua Biswas,** CSIR-National Chemical Laboratory, India

Proceedings Presentation: Resolving diverse protein-DNA footprints from exonuclease-based ChIP experiments

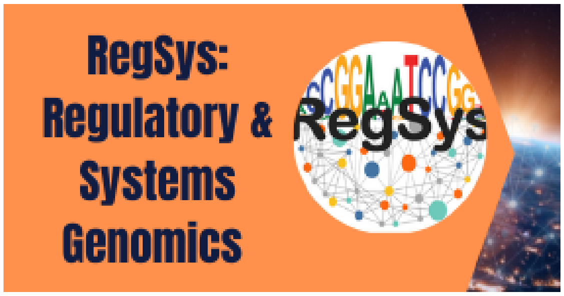
15:00 **Kelly Cochran,** Stanford University, United States

Domain adaptive neural networks improve cross-species prediction of transcription factor binding

REGSYS COSI

TRACK PRESENTATIONS

TUESDAY, JULY 27TH



11:00 **Anaïs Baudot**

COSI REGSYS KEYNOTE: Multi-omics data integration methods to study rare genetic diseases

11:40 **Aryan Kamal,** EMBL, Germany

Evaluating the predictive power of enhancer-mediated cell-type specific gene regulatory networks

12:00 **Yuning Zhang,** Center for Genomic and Computational Biology, Duke University, United States

Combining in vitro quantification with in vivo detection of protein-DNA interactions reveals subtle signals in gene regulatory networks

12:40 **Junha Shin,** Wisconsin Institute for Discovery, University of Wisconsin-Madison, United States

Characterizing the cellular diversity of early development of the human hindbrain and spinal cord

13:00 **Giacomo Corleone,** IRCCS Regina Elena National Cancer Institute, Italy

Mapping the DNA accessibility landscape of B-ALL patients revealed principles of cancer evolution.

13:20 **Liana Lareau,** University of California, Berkeley, United States

Identifying cell-state-associated alternative splicing events and their co-regulation

13:40 **Michael M. Hoffman,** University Health Network, Canada

Viral integration transforms chromatin to drive oncogenesis

14:20 **Olga Troyanskaya**

COSI REGSYS KEYNOTE: Regulation and human disease - from genome to networks

15:00 **Christopher Probert,** Stanford University, United States

Learning determinants of nucleosome positioning through sequence-based models of cell-free DNA

REGSYS COSI

TRACK PRESENTATIONS

WEDNESDAY, JULY 28TH

RegSys: Regulatory & Systems Genomics

11:00 **Camille Berthelot**

COSI REGSYS KEYNOTE: Tracing the evolution of gene regulation and the emergence of new traits

11:40 **Mathys Grapotte,** IGMM, France

Discovery of widespread transcription initiation at microsatellites predictable by sequence-based deep neural network

12:00 **Jian Zhou,** University of Texas Southwestern Medical Center, United States

Sequence-based modeling of genome 3D architecture from kilobase to chromosome-scale

12:40 **Juanma Vacquerizas**

COSI REGSYS KEYNOTE: Chromatin Conformation during Early Embryonic Development

13:20 **Zhanlin Chen,** Yale University, United States

Proceedings Presentation: DECODE: A Deep-learning Framework for Condensing Enhancers and Refining Boundaries with Large-scale Functional Assays

13:40 **Yangyang Hu,** University of California Riverside, United States

Proceedings Presentation: EnHiC: Learning fine-resolution Hi-C contact maps using a generative adversarial framework

14:20 **Yifeng Tao,** Carnegie Mellon University, United States

Interpretable deep learning for chromatin-informed inference of transcriptional programs driven by somatic alterations across cancers

14:40 **Dongyuan Song,** University of California, Los Angeles, United States

Proceedings Presentation: scPNMF: sparse gene encoding of single cells to facilitate gene selection for targeted gene profiling

15:00 **Irene Kaplow,** Carnegie Mellon University, United States

A Comparative Genomics Approach to Identifying Candidate Enhancers Associated with Phenotypes

iRNA COSI

TRACK PRESENTATIONS

WEDNESDAY, JULY 28TH

iRNA:
Integrative
RNA Biology

IRB
Integrative RNA Biology
group

11:00	**Manuel Irimia** ***iRNA Keynote: Parallel evolution of tissue-specific alternative splicing networks***
11:40	**Gabriela Santos Rodriguez,** Garvan Institute of Medical Research, Australia *Evolution of circular RNAs in primates*
12:00	**Michay Diez,** Stowers Institute for Medical Research, United States *iCodon: Harnessing mRNA stability to customize gene expression*
12:40	**Marie Coutelier,** Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Canada *When the silent genome gets loud: transcription of repeated genomic elements at single-cell resolution in tumours and along development*
13:00	**Pierre-Étienne Jacques,** Universitié de Sherbrooke, Canada *Identification and application of circulating microRNA expression quantitative trait loci (eQTL) at the first trimester of pregnancy*
13:20	**Mathieu Quesnel-Vallieres,** University of Pennsylvania, United States *Identifying universal cancer transcriptome patterns by interpreting deep learning models*
13:40	**Regan Hayward,** Helmholtz Institute for RNA-based Infection Research (HIRI), Germany *Improved quantification of host-pathogen dual RNA-seq experiments*
13:50	**Malindrie Dharmaratne,** University of Queensland, Australia *scShapes: A statistical framework for identifying distribution shapes in single-cell RNA-sequencing data*
14:20	**Wei Wang,** University of California, Los Angeles, United States *Proceedings Presentation: JEDI: Circular RNA Prediction based on Junction Encoders and Deep Interaction among Splice Sites*
14:40	**Carlos G. Oliver,** McGill University, Canada *Tools for the analysis of RNA 3D structures*
15:00	*Poster flash talks*

iRNA COSI

TRACK PRESENTATIONS

THURSDAY, JULY 29TH

iRNA:
Integrative
RNA Biology

IRB
Integrative RNA Biology
group

11:00 **Kathi Zarnack**
iRNA Keynote: Deep and accurate detection of m6A RNA modifications using miCLIP2 and m6Aboost machine learning

11:40 **Ruiyan Hou,** School of Biomedical Sciences, LKS Faculty of Medicine, The University of Hong Kong, China
Genomic sequences and RNA binding proteins predict RNA splicing kinetics in various single-cell contexts

12:00 **Salma Sohrabi-Jahromi,** Max Planck Institute for Biophysical Chemistry, Germany
Proceedings Presentation: Thermodynamic modeling reveals widespread multivalent binding by RNA-binding proteins

12:40 **Eddie Park,** Children's Hospital of Philadelphia, United States

Genetic variation and microRNA targeting of A-to-I RNA editing fine tune human tissue transcriptomes

13:00 **Pablo Acera,** Australian National University, Australia
Detection of RNA modifications at a single-molecule level using a two-stage deep learning model with Nanopore sequencing

13:20 **Sara H Rouhanifard,** Northeastern University, United States
Identification of Pseudouridine Modifications in mRNAs using Direct, Long-read Sequencing

13:40 **Daiyun Huang,** Xi'an Jiaotong-Liverpool University, China

Proceedings Presentation: Weakly supervised learning of RNA modifications from low-resolution epitranscriptome data

14:20 **Christoph Dieterich,** University Hospital Heidelberg, Germany
RNA modification mapping on the Illumina or Nanopore platform with JACUSA2

14:40 **Nicole Martinez, Shengdong Ke, Schragi Schwartz**

Panel discussion on epitranscriptomics

17:30 *Social hour*

iRNA COSI

TRACK PRESENTATIONS

FRIDAY, JULY 30TH

iRNA:
Integrative
RNA Biology

IRB
Integrative RNA Biology
group

11:00 **Liang Huang,** Oregon State University; United States
iRNA Keynote: Understanding RNA function through structure

11:40 **Samer Hussein,** Université Laval, Canada
Unravelling the function of Tapir lncRNA in regulating pluripotent cell states

12:00 **Danny Bergeron,** Université de Sherbrooke, Canada

RNA-RNA interaction network unravels gene regulation by embedded snoRNAs

12:40 **Xin Lai,** Universitätsklinikum Erlangen, Germany

Network- and systems-based re-engineering of dendritic cells with microRNAs for cancer immunotherapy

12:50 **Ana Conesa,** University of Florida, United States
SQANTI3: A collaborative project for curation, annotation and quantification of long reads RNA sequencing (lrRNA-seq) data

13:00 **Alla Mikheenko,** Saint Petersburg State University, Russia

Sequencing of individual barcoded cDNAs on Pacific Biosciences and Oxford Nanopore reveals platform-specific error patterns

13:20 **Athanasios Zovoilis,** University of Lethbridge, Canada

NERD-seq: A Nanopore direct RNA sequencing approach for non-coding RNAs

13:40 **Matthew Gazzara,** University of Pennsylvania, United States
Yuk Kei Wan, A-Star Institute, Singapore

APAeval: A community effort to benchmark tools for alternative polyadenylation

13:50 **Michelle Meyer,** Boston College, United States

The RBP Footprint Grand Challenge at RNA 2021-2022

14:20 **Liang Huang,** School of EECS, Oregon State University, USA

iRNA Keynote:Linear-Time Algorithms for RNA Folding and mRNA Design to Fight COVID-19

15:00 **Chengxin Zhang,** Yale University, United States

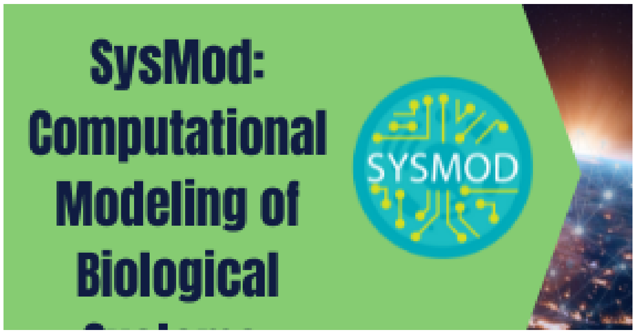
rMSA: accurate multiple sequence alignment generation to improve RNA structure modeling

15:10 *Closing remarks*

SYSMOD COSI

TRACK PRESENTATIONS

THURSDAY, JULY 29TH



11:00 **Claudine Chaouiya**
Introduction to the First SysMod 2021 Day

11:05 **Ines Thiele**
Whole-body metabolic modelling provides novel insight into host-microbiome crosstalk

11:50 **Reihaneh Mostolizadeh,** University of Tübingen, Germany
Workflow for modeling microbial community interactions applied to Dolosigranulum pigrum and Staphylococcus aureus within the human nose

12:05 **Paul Lang, University of Oxford**
BpForms and BcForms: a toolkit for concretely describing non-canonical polymers and complexes to facilitate global biochemical networks

12:40 **Marco Ruscone,** Curie Institute, France

Multiscale model of the different modes of invasion

12:55 **Eirini Tsirvouli,** Norwegian University of Science and Technology, Norway
Logical and experimental modeling of keratinocytes provide new insights in psoriasis and its treatment.

13:10 **Cedric Lhoussaine,** Univ. Lille, France
Limits of a Glucose-Insulin Model to Investigate Intestinal Absorption in Type 2 Diabetes

13:25 **Bhanwar Lal Puniya,** University of Nebraska-Lincoln, United States
Metabolic drug repurposing for autoimmune diseases

13:40 **Anna Niarakis**
Round table discussion and summary

14:20 **Jordan J.A. Weaver,** University of Pittsburgh, United States
Multicellular Spatial Model of RNA Virus Replication and Interferon Responses Reveals Factors Controlling Plaque Growth Dynamics

14:35 **Lauren Benoodt,** University of Rochester School of Medicine and Dentistry, United States
STREGA-NONA: Single-cell Transcriptomics Reveal Extended Gene-set Associations in Networks Optimized with a geNetic Algorithm

14:50 **Dawson D. Payne,** University of Virginia, United States
An updated genome-scale metabolic network reconstruction of Pseudomonas aeruginosa PA14 to characterize mucin-driven shifts in bacterial metabolism

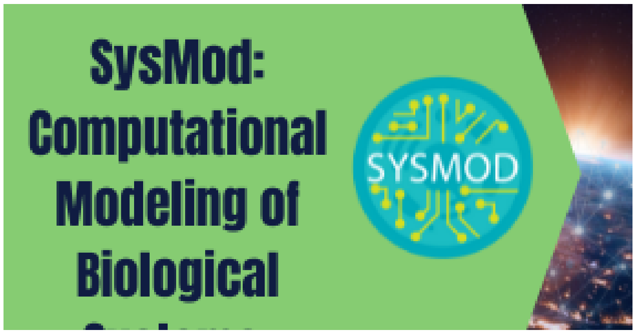
15:05 **Sanjeev Dahal,** Queen's University, Canada

Genome-scale modeling of Pseudomonas aeruginosa PA14 unveils broad metabolic capabilities and role of metabolism in virulence and drug potentiation

SYSMOD COSI

TRACK PRESENTATIONS

FRIDAY, JULY 30TH



11:00 **Laurence Calzone**
Introduction to the Second SysMod 2021 Day

11:05 **Ruth E. Baker**
Identifiability and inference for models in mathematical biology

11:50 **Nantia Leonidou,** Institute for Bioinformatics and Medical Informatics (IBMI),Germany
Tissue-specific reconstruction of constraint-based metabolic models based on ReconX

12:05 **Melania Nowicka,** Freie Universiteat Berlin, Germany
Designing distributed cell classifier circuits with genetic algorithms and logic programming

12:40 **Miroslav Phan, ETH Zurich, Switzerland**

A Rejection based Gillespie Algorithm for Non-Markovian Stochastic Processes

12:55 **Emilee Holtzapple,** University of Pittsburgh, United States
A data-driven Glioblastoma stem cell model provides insight into cell line differences in treatment resistance

13:10 **Maurício Moreira-Soares,** University of Oslo, Norway
Two models, same result: adhesion as key modulator for cell migration under confinement

13:25 **Marzia Di Filippo,** University of Milano-Bicocca, Italy
A model-based data integration pipeline to characterize the multi-level regulation of cell metabolism

13:40 **Matteo Barberis,** University of Surrey, United Kingdom
A novel and robust molecular design synchronizing transcription with cell cycle dynamics in budding yeast

13:55 **Matteo Barberis**

Discussion summary

14:20 **Boris N. Kholodenko**
Structure-based dynamic modeling reveals ways to overcome kinase inhibitor resistance and oncogenic RAS signaling and oncogenic RAS signaling.

15:05 **Juilee Thakar**

Closing remarks of SysMod 2021 and Poster Award

Text Mining COSI

TRACK PRESENTATIONS

WEDNESDAY, JULY 28TH

Text Mining for Healthcare and Biology

Mining

11:00 **Sampo Pyysalo,** University of Turku, Finland

Text Mining Keynote

11:40 **Arjun Krishnan,** Michigan State University, United States

Systematic tissue annotations of –omics samples by modeling unstructured metadata

12:00 **Paola Turina,** University of Bologna, Italy

ThermoScan: A text-mining approach for the identification of thermodynamic data on protein folding from full-text articles

12:10 **Matthew Artuso,** Michigan State University, United States

Quantifying general and discipline-specific word understandability towards better science communication

12:40 **Lynette Hirschman, Robert Ball**

Text Mining Keynote: Text Mining for Drug Safety at FDA: Autonomous Machines vs Human-in-the-Loop

13:20 **Maaly Nassar,** EMBL-EBI, United Kingdom

A machine learning framework for discovering and enriching metagenomics metadata from open access research articles

13:40 **Phillip Richter-Pechanski,** Klaus Tschira Institute for Integrative Computational Cardiology, Heidelberg, Germany

Automatic Extraction of Twelve Cardiovascular Concepts from German Discharge Letters using Pre-trained Language Models

14:20 **Pengyuan Li,** University of Delaware, United States

Proceedings Presentation: Utilizing Image and Caption Information for Biomedical Document Classification

14:40 **Zhiyong Lu,** NCBI, NLM, NIH, USA

Spotlight on Practical Text Mining Tools: LitSuggest & TeamTat

15:00 **Hoifung Poon**

Spotlight on Practical Text Mining Tools: PubMedBERT

TRANSMED COSI

TRACK PRESENTATIONS

SUNDAY, JULY 25TH

11:00 **Venkata Satagopam**

Opening

11:05 **Jochen Klucken**
TransMed Keynote: Personalized HealthTech Services: from data-driven innovation to Patient-centered Healthcare Application

11:40 **Peter Peneder,** St. Anna Children's Cancer Research Institute (CCRI), Austria
Multimodal analysis of cell-free DNA whole genome sequencing for pediatric cancers with low mutational burden

12:00 **Ilyes Baali,** Antalya Bilim University, Turkey
DriveWays: A Method for Identifying Possibly Overlapping Driver Pathways in Cancer

12:40 **Jean Clemenceau,** Cleveland Clinic, United States
Analyzing spatial heterogeneity of tumor mutation burden and immune infiltrates on whole slide images signals correlation with bladder cancer survival

13:00 **Konstantin Okonechnikov, Hopp Children's Cancer Center Heidelberg (KiTZ), Germany**
Analysis of single nucleus transcriptome profiles from developing human cerebellum reveals potential cellular origins of pediatric brain tumors

13:10 **Aissa Houdjedj,** Antalya Bilim University, Turkey
Ranking Cancer Drivers via Betweenness-based Outlier Detection and Random Walks

13:20 **Tiago Pereira,** University of Coimbra, Portugal
Proceedings Presentation: Optimising Blood-Brain Barrier Permeation through Deep Reinforcement Learning for De Novo Drug Design

13:40 **Kewalin Samart,** Michigan State University, United States
Reconciling Multiple Connectivity Scores for Drug Repurposing

14:20 **Jesus De la Fuente Cedeño,** TECNUN, University of Navarra, Spain., Spain
Identification of transcriptional network disruptions in drug-resistant prostate cancer with TraRe

14:40 **Sepideh Sadegh,** TUM School of Life Sciences Weihenstephan, Germany
NeDRex - an integrative and interactive network medicine platform for drug repurposing

15:00 **Yun Hao,** University of Pennsylvania, United States
A novel feature selection pipeline for identifying predictive targets associated with drug toxicity

15:10 *Closing of Day 1*

TRANSMED COSI

TRACK PRESENTATIONS

MONDAY, JULY 26TH

11:00 **Serena Scollen**
TransMed Keynote: Towards cross-border access to beyond one million sequenced human genomes

11:40 **Dillon Aberasturi,** The University of Arizona, United States
Proceedings Presentation: "Single-subject studies"-derived analyses unveil altered biomechanisms between very small cohorts: implications for rare diseases

12:00 **Meemansa Sood,** Fraunhofer SCAI and University of Bonn, Germany
Assessing the role of Digital Device Technology in Alzheimer's Disease using Artificial Intelligence

12:40 **Riya Gupta,** Center for Biomedical Informatics Research, United States
Formulating a Gene Signature for Diagnosis of Autoimmune and Infectious Diseases

13:00 **Ziye Tao,** University of Toronto, Canada
Proceedings Presentation: Expected 10-anonymity of HyperLogLog sketches for federated queries of clinical data repositories

13:20 **Colin Birkenbihl,** Fraunhofer SCAI, Germany
Synthesizing realistic patient-level data using multimodal neural differential equations

13:40 **Marius Herr,** University Hospital Tübingen & University of Tübingen, Germany
Bringing the Algorithms to the Data - Secure Distributed Medical Analytics using the Personal Health Train

14:20 **Kenneth Mandl**
TransMed Keynote: 21st Century healthcare is bringing computation to the bedside

15:00 **Nimrod Rappoport,** Tel Aviv University, Israel
MONET: Multi-omic module discovery by omic selection

15:10 *Closing*

VarI COSI

TRACK PRESENTATIONS

THURSDAY, JULY 29TH

11:00 **Emidio Capriotti, Hannah Carter, Antonio Rausell**
Opening Remarks

11:10 **Alessandra Carbone,** Sorbonne Universite, France
VarI Keynote: Mutations in viruses and humans.

12:00 **Chirag Jain,** Indian Institute of Science, India

Proceedings Presentation: A variant selection framework for genome graphs

12:40 **Abhirami Ram,** TCS Research, India

Identifying Factors Important for Conservation at Sites of Synonymous Variation

12:50 **Bian Li,** Vanderbilt University, United States

The structural landscape of constrained sites in the human proteome

13:10 **Ben Lehner**

VarI Keynote: Pan-genomic advances for fighting reference bias

14:20 **Joanna von Berg,** University Medical Center Utrecht, Netherlands
PolarMorphism enables discovery of genetic variants with shared effect across multiple traits from GWAS summary statistics

14:40 **Elena Bernabeu,** The University of Edinburgh, United Kingdom
Sex differences in genetic architecture in UK Biobank

14:50 **Yingying Wei,** The Chinese University of Hong Kong, Hong Kong
Identification of Ethnicity-Specific Associations in Multi-Ethnic Genome-Wide Association Studies

15:00 **Meghana Pagadala,** UCSD, United States
Germline variants that influence the tumor immune microenvironment also drive response to immunotherapy

VarI COSI

TRACK PRESENTATIONS

FRIDAY, JULY 30TH

11:00	**Ben Langmead** ***VarI Keynote: Sequence to energy and structure.***
11:50	**Joseph Ng,** King's College London, United Kingdom *Protein structural consequences of DNA mutational signatures: A meta-analysis of somatic variants and deep mutational scanning data*
12:10	**Giulia Babbi,** University of Bologna - Biocomputing Group, Italy *Physico-chemical and structural features of pathogenic and benign human protein missense variations collected from HUMSAVAR and ClinVar*
12:40	**Alexander Kaplun,** Variantyx, USA ***VarI Sponsor: A unique solution to a (non) unique problem: calling variants in non-uniquely mappable regions using short-read WGS data.***
12:55	**Yana Bromberg, Douglas Fowler, Daniel Gilchrist, Predrag Radivojac** *VarI Roundtable*
14:20	**Steven E. Brenner,** University of California, Berkeley, United States ***The role of exome sequencing in newborn screening***
14:30	**Marc Vaisband,** Salzburg Cancer Research Institute, Germany *Validation of genetic variants from NGS data using Deep Convolutional Neural Networks*
14:40	**Martin Kircher,** Berlin Institute of Health @ Charité, Germany *CADD-SV -- a framework to score the effects of structural variants in health and disease*
15:00	**Francisco Requena,** Imagine Institute for Genetic Diseases, France *CNVxplorer: a web tool to assist clinical interpretation of CNVs in rare disease patients*
15:10	**Stephen Yi,** University of Texas at Austin, United States *Emerging gain-of-function mutations in disease: their computational interpretation and characterization*

TECHNOLOGY TALK

PRESENTATIONS

FRIDAY, JULY 30TH

11:00 **Michael J Sternberg,** Imperial College London, United Kingdom

Phyre2 and Missense3D: Protein structure prediction and missense variant analysis

11:20 **Ian Sillitoe,** University College London, United Kingdom

Using CATH-Gene3D v4.3 and its resources to predict the structure and function of novel protein sequences

11:40 **Santiago Nicolas Lopez Caranza,** InstaDeep, United Kingdom

DeepChain: A platform for protein design

12:00 **Renato Alves,** de.NBI - German Network for Bioinformatics Infrastructure, Germany

Developing a reusable and versatile virtual bioinformatics training platform in the de.NBI cloud

12:40 **Fabio Madeira,** European Bioinformatics Institute, United Kingdom

The EMBL-EBI search and sequence analysis tools APIs and their role during the current COVID-19 pandemic

13:00 **Raheela Aslam,** EMBL-EBI, United Kingdom

The European COVID-19 Data Portal – Accelerating COVID-19 Research through Open Data Sharing

13:20 **Jose Carbonell,** Barcelona Supercomputing Center, Spain

PerMedCoE: A roadmap to scalability in Personalized Medicine

14:20 **Michael Reich,** UCSD, United States

The GenePattern Notebook Environment

14:40 **Peter Karp,** SRI International, United States

Integrated Pathway/Genome/Omics Informatics in Pathway Tools and BioCyc

NIH/OD OFFICE OF DATA SCIENCE STRATEGY (ODSS)

PRESENTATIONS

ISMB/ECCB 2021
Special Sessions

TUESDAY, JULY 27TH

11:00	**Susan Gregurick** *Session I: The NIH Cloud Platforms Interoperability (NCPI) Efforts*
11:00	**Susan Gregurick** *Welcome and Introduction*
11:10	**Brian O'Connor** *Federated and FAIR Systems Interoperation in NCPI*
11:33	**Allison P Heath** *Clinical and Phenotypic Data Interoperability using FHIR in NCPI*
11:56	**Michael C. Schatz** *Modeling the computing requirements and costs for genomics analysis in the cloud*
12:40	**Jennie Larkin & Ishwar Chandramouliswaran** *Session II: FAIR Data/Repositories*
12:40	**Ishwar Chandramouliswaran,** NIAID/NIH, USA *NIH Activities to Support a FAIR Repository Ecosystem*
12:45	**Mark Hahnel** *FAIR Research - What is in it for the Researchers?*
13:00	**Lara Mangravite** *The Tribal Nature of Data Sharing*
13:15	**John Chodacki,** California Digital Library (CDL), USA *FAIR Data and FAIR Repositories*
13:30	**Carole Goble,** The University of Manchester / ELIXIR-UK *Bridging from Researcher Data Management to ELIXIR Archives in the RDM Lifecycle*
13:45	**Sandra Tang** *An Introduction to ICPSR: A Place to Discover and Access Social and Behavioral Science Data for Secondary Analysis*
14:20	**Susan Gregurick** *Session III (Panel): Diversity in Data Science Training and Research*

NIH/OD OFFICE OF DATA SCIENCE STRATEGY (ODSS)

PRESENTATIONS

WEDNESDAY, JULY 28TH

11:00 **Heidi Sofia**

Session IV: Open Research Software

11:00 **Susan Gregurick**

Welcome and Introduction

11:05 **Alfredo Morales Pinzon,** Brigham and Women's Hospital & Harvard Medical School, USA

Manual Brain Segmentation Workflows Using the SPINE Virtual Laboratory: from Desktop to Cloud

11:20 **Laurel Carney**

UR_EAR - A Web App supporting computational models for auditory-nerve and midbrain responses

11:35 **Ajay Dharod**

mPATH: A Digital Health Navigator

11:50 **Pinaki Sarder,** University at Buffalo, USA

Human AI Loop in Cloud for Distributed Computation

12:05 **Jeff Wagner,** Open Force Field Initiative, USA

Software and Science at the Open Force Field Initiative

12:40 *Session V: Reproducibility & Re-use*

12:40 **Alex Bui**

Introduction and Welcome

12:44 **Nigam Shah,** Stanford University, United States

A Framewok for Making Predictive Models Useful in Medicine

13:03 **Bin Yu**

Veridical Data Science for precision medicine: subgroup discovery through staDISC

13:22 **Anders O Garlid**

PREMIERE: A community-driven platform for reproducibilty and reuse in biomedical predictive modeling

13:41 **Yasset Perez-Riverol**

Omics Indexing and Standards

14:20 **Michele Ramsay, Claudia Medeiros, Chuck Cook, Griffin M. Weber,** Harvard Medical School, United States

Session VI (Panel): Bridging International Efforts in Data Science

WEB 2021: MAKING TRAINING MATERIALS FAIR - EXPERIENCES, CHALLENGES, SOLUTIONS

SUNDAY, JULY 25TH

This workshop is organised and supported by **GOBLET**, the Global Organisation for Bioinformatics Learning, Education and Training and the **ISCB Education COSI**.

11:00 **Patricia Palagi,** SIB Swiss Institute of Bioinformatics, Switzerland
Welcome and introductions

11:15 **Melissa Burke,** Australian BioCommons, Australia
Making training FAIR in ten simple rules

11:30 **Sarah Morgan,** EMBL-European Bioinformatics Institute, United Kingdom
The CINECA Hackathon report

11:40 **Saskia Hiltemann,** Erasmus Medical Center, The Netherlands
Experiences from the Galaxy Training Network

11:47 **Anna Swann,** EMBL-European Bioinformatics Institute, United Kingdom
Experiences from the EMBL-European Bioinformatics Institute

11:54 **Verena Ras,** University of Cape Town, South Africa
Experiences from the H3ABioNet

12:01 **Maria Doyle,** Peter MacCallum Cancer Centre, Australia
Experiences from an Individual Trainer

12:08 *Q&A*

12:40 **Melissa Burke,** Australian BioCommons, Australia
Experiences from the Australia BioCommons

12:47 **Patricia Palagi,** SIB Swiss Institute of Bioinformatics, Switzerland
Experiences from the SIB Swiss Institute of Bioinformatics

12:54 **Celia van Gelder,** DTL Dutch Techcentre for Life Sciences, The Netherlands
Experiences from the OpenAIRE Community of Practice for training coordinators

13:01 *Q&A*

13:06 **Melissa Burke, Celia van Gelder, Patricia Palagi**
Group discussion: Identifying challenges and issues

14:20 **Melissa Burke, Celia van Gelder, Patricia Palagi**
Group discussion: Identifying solutions to ease FAIRyfication of training materials

14:55 *Reporting Back*

15:15 **Celia van Gelder,** DTL Dutch Techcentre for Life Sciences, The Netherlands
Closing remarks

COLLABORATIVE TOOLS FOR PROTEIN ANALYSIS HACKATHON 2021

THURSDAY, JULY 29, 12:40 - 14:00 UTC

Final Project Presentations and Discussion

Towards integrating protein sequence-structure-function analysis, visualization and open collaborative research

The two main goals of this virtual hackathon are:

To develop open source software modules and collaboration tools for universal biomolecular analyses enabling integration of diverse knowledge and datasets.
To create a sustainable diverse community of developers and designers for continued development of such tools

SCIENCE COMMUNICATION AND SCIENCE JOURNALISM

TUESDAY, JULY 27

Moderator: Thomas Lengauer, Past President, ISCB

Panelists:
Kai Kupferschmidt, Independent Science Journalist
Emma Hodcroft, University of Bern
John Moult, Institute for Bioscience and Biotechnology Research (IBBR) , University of Maryland
Freya Robb, Science Media Centre

The COVID-19 pandemic has brought science into the limelight of public perception in an unprecedented fashion. Scientists have become more present in the media, accelerated transmission of new results has been effected by the public starting to pay attention to research reports that have not been reviewed yet, journalists have been faced with the requirement to bring such emerging results to the public at short notice. This process has also fed an increased controversy on the character of science and the role it does and should play in the public discourse.

In this panel, a science journalist and a science communicator will join two scientists to discuss issues on how to best effect communication to the public on science results and also and especially on the science process.

SEE YOU NEXT YEAR IN PERSON FOR ISMB 2022 IN MADISON, WISCONSIN!

JULY 10 - 14, 2022

https://www.iscb.org/ismb2022

Mark Your Calendars

iSCB
INTERNATIONAL SOCIETY FOR
COMPUTATIONAL BIOLOGY

iSCB
ISMB
2022
MADISON
JULY 10–14

JOIN US AT THE PREMIER COMPUTATIONAL BIOLOGY MEETING OF THE YEAR!
DISCOVER, INNOVATE AND CONNECT

MEET YOUR
ISCB BOARD OF DIRECTORS

ISCB EXECUTIVE OFFICERS & DIRECTORS

Christine Orengo, Ph.D.
President, ISCB
Professor
University College London
UNITED KINGDOM

Thomas Lengauer, Ph.D.
Immediate Past-*President, ISCB*
Prof. Dr.
Max Planck Institute for Informatics
GERMANY

Alex Bateman, Ph.D.
Vice President, ISCB
Head of Protein Sequence Resources
EMBL- EBI
UNITED KINGDOM

Yana Bromberg, Ph.D.
Vice President, ISCB
Associate Professor
Rutgers University
USA

Terry Gaasterland, Ph.D.
Vice President, ISCB
Professor
University of California San Diego
USA

Bruno Gaeta, Ph.D.
Treasurer, ISCB
Senior Lecturer and
Bioinformatics Program Director
University of New South Wales
AUSTRALIA

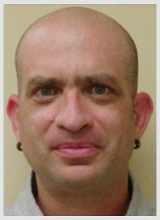
Michelle Brazas, Ph.D.
Secretary, ISCB
Senior Program Manager
Ontario Institute for Cancer Research
CANADA

ISCB BOARD OF DIRECTORS

Bonnie Berger, Ph.D.
Professor
Applied Mathematics and
Computer Science
MIT
USA

Catherine Brooksbank, Ph.D.
Head of Training
EMBL-EBI
UNITED KINGDOM

Christophe Dessimoz, Ph.D.
Prof.
University of Lausanne
SWITZERLAND



Iddo Friedberg, Ph.D.
Associate Professor
Iowa State University
USA

Wataru Iwasaki, Ph.D.
Associate Professor
The University of Tokyo
JAPAN

Janet Kelso, Ph.D.
Group Leader
MPI for Evolutionary Anthropology
GERMANY

Scott Markel, Ph.D.
R&D Development Director,
Scientific Services
Dassault Systèmes BIOVIA
USA

MEET YOUR
ISCB BOARD OF DIRECTORS

Tijana Milenkovic, Ph.D.
ISCB COSI Representative to the Board,
Frank M. Freimann Collegiate Associate
Professor of Engineering
University of Notre Dame
USA

Yves Moreau, Ph.D.
Professor
KU Leuven
BELGIUM

Farzana Rahman, Ph.D.
Student Council Representative,
Lecturer in Bioinformatics, Canterbury
Christ Church University
Visiting Research Fellow,
University of South Wales
UNITED KINGDOM

Christian Schönbach, Ph.D.
Affiliates Group Representative, ISCB
Professor
Nazarbayev University
KAZAKHSTAN

Russell Schwartz, Ph.D.
Professor
Carnegie Mellon University
USA

Hagit Shatkay, Ph.D.
Professor
University of Delaware
USA

Saurabh Sinha, Ph.D.
ISCB COSI Representative to the Board,
Professor
University of Illinois
USA

Alfonso Valencia, Ph.D.
PROFESSOR
Barcelona Supercomputing Center -
Centro Nacional de Supercomputacion
(BSC)
SPAIN

Mark Wass, Ph.D.
COSI Representative to the Board, ISCB
Reader in Computational Biology
University of Kent
UNITED KINGDOM

Xuegong Zhang, Ph.D.
Professor
Tsinghua University
CHINA

upcoming

EVENTS OF INTEREST

INTERNATIONAL SOCIETY FOR COMPUTATIONAL BIOLOGY

RECOMB 2021

Aug 29, 2021 through Sep 01, 2021

https://www.iscb.org/cms_addon/events/details.php?uid=2874

3rd International Symposium on Mathematical and Computational Oncology (ISMCO'21)

Oct 11, 2021 through Oct 13, 2021

https://www.iscb.org/cms_addon/events/details.php?uid=2896

BBCC 2021 - Bioinformatics and Computational Biology Conference

Dec 01, 2021 through Dec 03, 2021

https://www.iscb.org/cms_addon/events/details.php?uid=2914

ROCKY 2021

Dec 02, 2021 through Dec 04, 2021

https://www.iscb.org/rocky2021

Pacific Symposium on Biocomputing (PSB) 2022

Jan 03, 2022 through Jan 07, 2022

https://www.iscb.org/cms_addon/events/details.php?uid=2887

ISCBacademy Webinar Series

- Registration free for ISCB members
- Watch archived talks
- Propose an idea for a webinar

https://www.iscb.org/iscbacademy-webinars

ISCB Officers and Executive Committee

Christine Orengo, Ph.D.
President
Thomas Lengauer, Ph.D.
Immediate Past-President
Alex Bateman, Ph.D.
Vice President
Yana Bromberg, Ph.D.
Vice President
Terry Gaasterland, Ph.D.
Vice President
Bruno Gaeta, Ph.D.
Treasurer
Michelle Brazas, Ph.D.
Secretary

ISCB Board of Directors

Alex Bateman, Ph.D.
Bonnie Berger, Ph.D.
Michelle Brazas, Ph.D.
Yana Bromberg, Ph.D.
Catherine Brooksbank, Ph.D.
Christophe Dessimoz, Ph.D.
Iddo Friedberg, Ph.D.
Terry Gaasterland, Ph.D.
Bruno Gaeta, Ph.D.
Wataru Iwasaki, Ph.D.
Janet Kelso, Ph.D.
Thomas Lengauer, Ph.D.
Scott Markel, Ph.D.
Tijana Milenkovic, Ph.D.
Yves Moreau, Ph.D.
Christine Orengo, Ph.D.
Farzana Rahman, Ph.D.
Christian Schönbach, Ph.D.
Russell Schwartz, Ph.D.
Hagit Shatkay, Ph.D.
Saurabh Sinha, Ph.D.
Alfonso Valencia, Ph.D.
Mark Wass, Ph.D.
Xuegong Zhang, Ph.D.

ISCB Staff

Diane E. Kovats, CAE, CMP, DES
Chief Executive Officer
Nadine Kampman Costello
Marketing and Communications Manager
Belinda (Bel) Humes Hanson, CMP
Operations and Programs Senior Manager
Seth Munholland, Ph.D.
Operations and Programs Specialist

WWW.ISCB.ORG

CONNECTING, TRAINING, EMPOWERING, WORLDWIDE