

Friends of GST,

*All Blues, Miles Davis, 1959*

No auspicious celestial event in 2019? This year's solar eclipse mostly traveled across the South Pacific. 'So what' you say. Speaking of which, coinciding with the start of the fall semester is the 60th anniversary of Miles Davis's pivotal album *Kind of Blue*, whose release ushered in an entirely new style of jazz. As in music, in science the significant inflection points are only obvious in retrospect.

This year, we are mourning the loss of our faculty colleague Dr. Elizabeth (Liz) Howell who passed away April 9 of this year. A decorated enzymologist, Liz Howell was among the most active and committed GST faculty members serving in more ways than can be listed here, but perhaps nowhere more prominently than by instructing the grant-writing course. She also embodied life at the interface of art and science, writing and even teaching (!) poetry, painting, all the while weaving ever more intricate representations of her model system, the enzyme dihydrofolate reductase.

Are you looking for a path to the tidal flats and pools between art and science? Mark September 6-27 to attend the inaugural "Art of Science" exhibit at the Emporium Center, 100 S. Gay Street. To be displayed are 3D and 2D works as well as videos and projections. Co-organized by Tessa Burch-Smith and Elena Ganusova, its premise is that the perspective of the artist can be a conduit to engage with original scientific inquiry. Go for it! The idea that contemporary art has a place in contemporary technology was a cornerstone of the 'Bauhaus' school of architecture and design, which was founded exactly 100 years ago. As we enter the age of synthetic biology, it stands to reason that artistic expression will eventually come to embellish the purely functional designs of bio-engineered systems as well.

GST students certainly seem to be well equipped to 'carpe diem', grasp these and other emergent opportunities. Overleaf you find reports on GST students attending an X-ray crystallography workshop at Cold Spring Harbor Labs, a computing workshop at the Pittsburgh Supercomputing

Center, and an internship in machine learning at a biotechnology company. Lining up these opportunities does take some investment, and the necessary cooperation to make it happen is easiest to obtain if progress towards the degree has been at least satisfactory, but the reports below also speak of ample rewards!



Artwork by Liz Howell. Here, a variation on Wassily Kandinsky's sketches "Farbstudie Quadrate" is setting the stage for structural models of dihydrofolate reductase. Of note, Kandinsky was a member of the Bauhaus.

In March of 2019, the GST community gathered at the annual retreat. Students hosted two of our many successful alumni. Brian Erickson shared his experience of starting a proteomics service company out of his postdoc at Harvard Medical School. Tatiana Nanda presented her insights from a career in the pharmaceutical industry, most recently at Johnson & Johnson. Their perspectives and advice, freely shared, was refreshing and lifted the veil of mystery from various career development questions.

All Blues? Not quite.

With best wishes for an academic year ripe with exciting discoveries,

*Albrecht v. Arnim*

Albrecht von Arnim

## AWARDS AND RECOGNITIONS WON BY GST STUDENTS

**Suresh Poudel** gave the Graduate Hooding Commencement speech on December 14 2018.

**Sarah Cooper** won the Cokkinias award from the Division of Biology

**Khushboo Bafna** received the College of Arts and Sciences Dissertation Fellowship Aug 2018-July 2019.

She was also cited for exceptional professional promise at the Chancellor's Honors Banquet in April 2019.

**Alexander Cope, Katrina Schlum, and Shantanu Shukla** each have a monetary award from the National Institute for Mathematical and Biological Synthesis

Nice going and congratulations!

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## FACULTY SPOTLIGHT: MICHAEL GILCHRIST

Dr. Michael Gilchrist is a GST faculty member in the Department of Ecology and Evolutionary Biology. His interdisciplinary research investigates the evolutionary consequences of molecular events at the level of protein synthesis. He builds computational models of protein synthesis for genome-scale bioinformatic datasets. He has advised a number of GST students, and most students know him for inserting a healthy dose of population and evolutionary genetics into the GST I core course.

**GT:** Thanks for carving out some time to share your perspective with our readers. Your work stands apart in our community in that it bridges between molecular processes, i.e. codon usage in translation, and population-level processes, specifically molecular evolution. Why do you think not many scientists (here) make this connection?

**MG:** That's an interesting question. Evolution and genetics have a long intertwined history dating back to the late 1800's. Indeed, I am always blown away by the fact that the foundations of evolutionary genetics were developed before scientists even knew genetic information was encoded in DNA and not proteins. But to get to your question, I think the reason most evolutionary biologists here don't focus on molecular processes reflects the history and culture of this field, which has primarily focused on the morphological and behavioral levels. My evolutionary biology colleagues here are happy to utilize genetic tools in their research; for example, to tell them about non-molecular processes such as the exchange of alleles between populations over time or the ultimate effect of genetic differences on reproduction and survival rather than the more fine scale, molecular implications of these differences.

In contrast, I think most molecular biologists have an oversimplified view of evolution as simply being all about natural selection and adaptation. This isn't a problem just in the field of molecular biology. This misguided view is quite widespread in other areas in biology and, indeed, used to plague the field of evolutionary biology decades ago. Biologists working under this misconception generally assume most things we observe in biology are there because they conferred some kind of adaptive advantage.

At the molecular level, this is often not the case and can lead to a very distorted view of biology. For example, it is very difficult to come up with a cogent adaptive explanation as

to why ~44% of the human (or really any mammalian) genome is made up of parasitic DNA (i.e. mobile genetic elements) but only 0.8% of it is made up of coding exons (regions that actually code for proteins). However, if we expand our evolutionary thinking to include the effects of genetic drift, we can begin to understand how ever so slightly deleterious DNA parasites could spread so widely across the mammalian genome.

**GT:** What is your pet project right now?

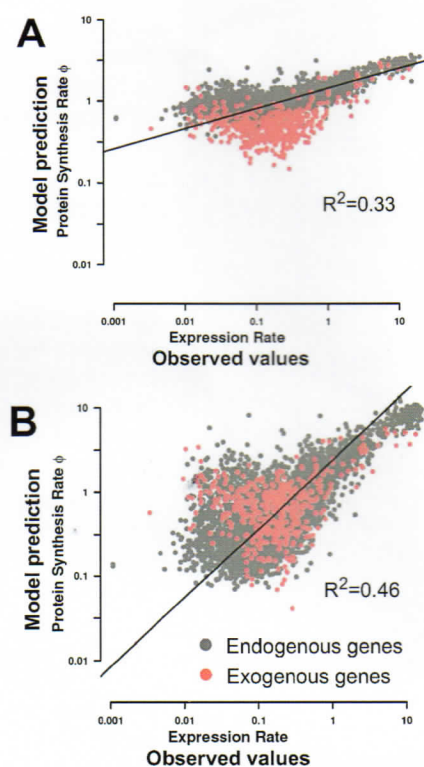
**MG:** One of my early interests in protein translation was the prevalence and cost of premature termination of protein translation or nonsense errors. Even after a decade, the evidence we have about their importance is limited, but it clearly supports the idea that ~20-30% of the time ribosomes terminate translation prematurely. Because we lack high quality estimates of how these error rates vary between synonymous codons, the overall influence of these nonsense errors on codon usage bias is still unclear. We've recently made some advances in our modeling that should allow us to estimate these errors directly from empirical ribosome footprinting data and I think we are close to being able to estimate them from genome sequence data. I'm looking forward to seeing how well the estimates from these two methods match up.

**GT:** Your work also stands out because it combines both mathematical modeling and large 'bioinformatics' datasets. Where is this field headed and how do we best prepare PhD students for success at this interface?

**MG:** The field of bioinformatics is growing in leaps and bounds. This is largely driven by the fact that empiricists keep pushing the boundaries of data collection forward, this is especially true for molecular data. The challenge is how to make sense of all of this data or, more precisely, how do we extract and contextualize the meaningful biological information in the data. There are many ways to do this, some are better than others. I focus my student training on the three fundamental skills that feedback to one another: biological knowledge, mathematical model building, and computational model fitting. You need to have a basic understanding of the biology in order to properly model what the data represents, you also need to understand how foundational ideas in probability can be used to fit these models to the data, the biological knowledge then comes back to the fore when you look at the results of your model fits.



Photo credit: Spencer Barrett



ROC-SEMPPR model predictions of protein synthesis rates vs. observed values of gene expression for the yeast *Lachanea kluyveri*. In this species, due to an ancient hybridization event, introgressed genes in the left arm of chromosome C (exogenous genes, red dots) have a different pattern of codon usage than the rest of the genome (black dots). In (A) the model's prediction ignores this fact. In (B) a separate model was fitted to the hybridized region, substantially increasing the predictive quality of the model.



## INTERVIEW WITH MICHAEL GILCHRIST

How well does the model do in capturing the patterns in the data? Are the patterns as you predicted or, as is usually the case, how do they deviate from your expectations? What can you add to the model to try and explain away some of these deviations? My view is if you have a decent handle on the biology, math, and stats you can attack any problem.

**GT: We like to see collaborative projects between ORNL and UT, and you have been successful with threading this needle? What is your experience with making this work?**

**MG:** In my experience, collaborating with folks at ORNL isn't hard \*if\* you have bright,

motivated, curious, and driven graduate students or post-docs. These folks really serve as the glue for collaborations between principle investigators and this is where the GST program has really shined. By co-advising GST graduate students I've been able to develop very productive collaborations with folks at ORNL.

**GT: You are planning on an exciting new course this Fall. Please tell us about it.**

**MG:** The class is on the evolution of cancer and I apply our understanding of how evolution works at both the species and within-patient scales. The goal is to use our under-

standing of natural selection, mutation, and genetic drift to help us better understand: why cancer persists (despite reducing the fitness of those who develop it), the steps involved in the development of different types of cancer within a patient, and how all of this can be used to explain the prevalence of cancer as a function of patient age and help design better treatments. I've limited the enrollment to 20 students to help foster student inquiry as we explore these topics, so I think it's going to be an interesting course.

**GT: Thank you and all the best.**

## NEW GST FACULTY



**Dr. David Talmy** is an Assistant Professor in Microbiology and is associated with NIMBioS, the National Institute for Mathematical and Biological Synthesis. His expertise lies in the microbial ecology of the oceans at an ecosystem level, in particular the role of viruses in controlling phytoplankton populations as well as carbon and nitrogen cycling. He was originally trained as a mathematician and initiated his segue into ecology as a Master's student. He came to UT from a postdoc at MIT.



**Dr. Keerthi Krishnan** adds to the growing contingent of neuroscientists at UT, having been hired out of a postdoc at Cold Spring Harbor Laboratory into the Department of Biochemistry & Cellular and Molecular Biology. Dr. Krishnan studies mechanisms of neural development in mouse models. Her research seeks to understand the consequences for neural plasticity of inherited defects in the gene for methyl CpG binding protein2 (MECP2), the primary cause of Rett syndrome, an X-linked condition restricted to females. Her technical approach reaches from genomics all the way to behavioral assays.



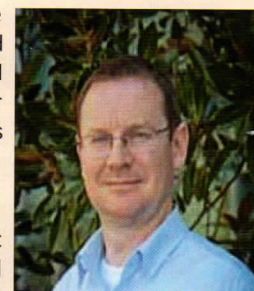
**Dr. Cong Trinh** is an Associate Professor in the Department of Chemical and Biomolecular Engineering at UT. He is a leader in the emergent field of synthetic biology where he combines experimentation and mathematical modeling especially for the metabolic engineering of bacteria that convert cellulosic biomass into biofuels. One core project has centered on the metabolic engineering of esters, which impart a wonderful smell to otherwise odorous bacteria. On the technical side, his lab is advancing CRISPR/Cas genome editing techniques for non-model organisms. He already has a distinguished record of PhD training, publication, and grantsmanship.



**Dr. Hugh O'Neill** is a Senior Staff Scientist at ORNL in the Neutron Science Division where he leads the initiative on "Biological Materials and Biosystems". He is an internationally recognized wet-lab biochemist with a strong track record of accomplishments in plant biochemistry primarily in the area of cell wall structure and function, as well as photosynthesis. Much of his work is in conjunction with computational molecular biophysicists and structural biologists. He has already collaborated extensively with researchers at UT. Dr. O'Neill has also advised PhD students through the Bredesen Center.



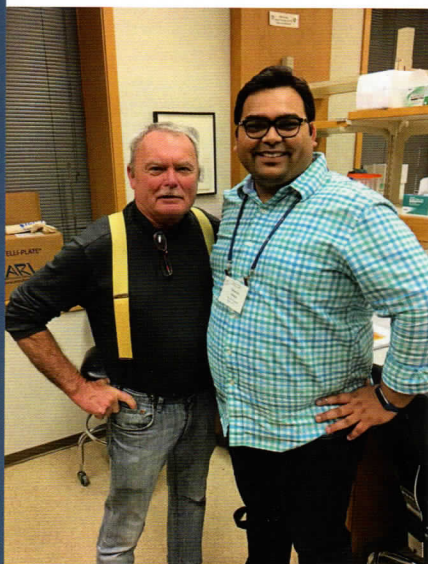
**Dr. Paul Abraham** is a Staff Scientist at ORNL in the Chemical Sciences Division, working in the proteomics group of Dr. Robert Hettich. Dr. Abraham is a resident expert on plant proteomics at ORNL and has primary experience in integrating omics data at different scales. He has gained deep insights into the proteins dynamics of plants such as Agave that are extremely well adapted to arid environments by way of a metabolic strategy known as Crassulacean Acid Metabolism. This work has been contrasted with other biofuel plants such as poplar trees. He has co-taught the mass spectrometry courses in GST with Dr. Hettich, and has worked extensively with GST students, and with research groups at UT. He is even an alumnus of the GST program.





## CRYSTAL PALACE

In October 2018, Shantanu Shukla (Myles lab) attended the course "X-Ray Methods in Structural Biology". Held annually at the Cold Spring Harbor Laboratory only 16 participants are selected out of a large plie of applicants to learn from leading figures in the field. Shantanu returned exhilarated having made new contacts including leads for postdoc opportunities.



Shantanu Shukla with course instructor, Prof. Alexander McPherson

**GT: I hear you really enjoyed the experience? What got you interested in attending the course?**

**SS:** My strongest motivation to apply was the willingness of the organizers to even accept students with no theoretical background in X-ray diffraction and scattering techniques. The other more obvious reason for me was to meet and attend lectures by pioneering scientists in the field of X-ray crystallography, like Prof. Alexander McPherson.

**GT: What were some of the benefits of attending?**

**SS:** CSHL courses are tailored in a way to address the very core and fundamental aspects of any research area. Given that the course program is spread across 15 days, one gets to revisit the same concepts over and over during both lecture and lab-based hands-on sessions. This reinforces the key concepts that are

required to perform the experiments correctly and to understand the quality of the data generated from those experiments. Besides, the student to instructor ratio is almost 1:1 so you get plenty of personal attention at this course. Students can even bring their own samples along, perform experiments on them, and get insights on their research projects from the instructors. Moreover, the biggest advantage of this course is the networking opportunity you get with some very prominent scientists and your peers, who are often early career researchers.

**GT: Did you get to do an experiment on your own project?**

**SS:** Yes, I took large deuterated crystals of my protein, which I collected diffraction datasets on at both Cold Spring Harbor Laboratory's X-ray diffractometer and at the National Synchrotron Light Source at the Brookhaven National Laboratory.

**GT: How did it change your thinking about your project or your career outlook?**

**SS:** It most certainly opened my eyes to a world full of possibilities in the field of Structural Biology. I got very good feedback from my peers and the mentors on my project involving neutron crystallography and scattering. As conceptually both X-ray and neutron crystallography apply the same principles of physics and mathematics, the knowledge gained at this course has helped me to design better neutron experiments for my system of interest.

**GT: What was the balance between theory and practice?**

**SS:** There is an equal distribution of time for both lectures and practical hands-on training, with lectures starting in the morning and early afternoon followed by lab-based work thereafter. Students were encouraged to work more than the actual on-paper time designated for lab work. All the instructors would hang around with the students in the lab everyday till almost 3 o'clock in the morning.

**GT: How did you fund your attendance?**

**SS:** My attendance was funded in part by

a generous scholarship from the National Institute of General Medical Sciences and by the Neutron Sciences Directorate, Oak Ridge National Laboratory.



**GT: What did you think about Cold Spring Harbor?**

**SS:** It is such a beautiful and serene place. The whole atmosphere was so energizing. We had a wonderful discussion session at the beach, which was very unique and fun-filled. On our day off, I went down to see the historic Sagamore Hills residence of late President Theodore Roosevelt. 15 days went by so fast at CSHL that I wish I could have stayed there for some more time.



View of Long Island Sound from Cold Spring Harbor Labs

**GT: Thank you, also for the inspiring photos.**

*An interview with Shantanu was also featured on the CSHL website at*

<https://currentexchange.cshl.edu/blog/2018/10/visitor-of-the-week-95>



## INTELLIGENT BIOFUEL FOR THE MACHINE LEARNING ENGINE

This summer, Yang Xu (McCord lab) is interning as a bioinformatics analyst at Engine Biosciences in the Bay area.

**GT: How did you come across this internship opportunity?**

YX: I am very interested to work in the biotech industry after graduation, and because I have zero experience with industry I felt an internship could ease what might otherwise be a hard transition. Last February I started to search for computational biology/ bioinformatics summer intern positions. Heads up: I think I sent out more than 50 resumes! I had six interviews, and luckily Engine Biosciences offered me a position in their bioinformatics division.

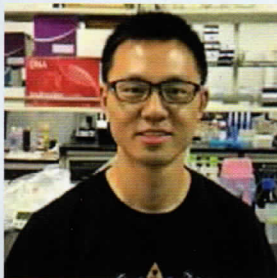
**GT: What is your internship project about?**

YX: The company's stated mission is 'Network Biomedicine for Drug Discovery'. I am working on biomedical text mining. In short, I am using machine learning to categorize biomedical publications and targeting specific cancer papers. Our goal is to train the machine to comprehend biomedical publications by deep learning. For example, if a gene/protein interaction is mentioned in the text, what type of interaction?

And in what scenarios, for example what cell line, pathway, genetic background, etc. Although this project isn't directly related to my dissertation project, I really appreciate that it exposes me to a new field where machine learning can come in to facilitate biomedical research.

**GT: What has been your experience so far?**

YX: My supervisor split the time into two phases and follows my progress every week. So far, we are close to the end of phase 1, which is categorization of publications and selection of specific papers. The next phase will be the hard part, but



we already came up with a plan to approach the problem. The working style is quite casual. My supervisor told me "Don't go to the office on Friday, because I work from home. You can do the same." That said, I do need to work extra hours if I fall behind schedule. I am also meeting very talented people here. The employees on the computational team have many years

of data science or machine learning experience.

**GT: Isn't there a wide gap between bioinformatics and drug discovery for the clinic?**

YX: Actually, the company consults closely with experts in the field, for example with oncologists from all over of the States. I had the opportunity to join a phone meeting with an oncologist from UCSF who specializes in lung cancer.

**GT: Would you recommend this kind of internship to other GST students?**

YX: Yes, strongly. The Bay area is a great place to live and work. Here is an interesting benefit that I did not consider before: Since the company is expanding I attended a few on-site interviews with job candidates. One person from Duke left a big impression on me. She conveyed a clear talk about her PhD research and gave convincing reasons why the skills she learned in grad school qualified her for the job. The way she delivered concepts and her passion during the talk inspired me how to sell myself as the right person to hire.

## RECENT CONFERENCES ATTENDED BY GST STUDENTS

**American Society for Mass Spectrometry Conference**, Atlanta, GA, July 2-7, 2019; Ivan Villalobos Solis, Samantha Peters, Alfredo Blakeley-Ruiz, Chen Cheng, Payal Chirania, Him Shrestha (all Hettich lab).

**Southeast Enzyme Conference**, Atlanta, GA, April 12-13, 2019; **Experimental Biology Conference**, Orlando FL April 04-09, 2019; Khushboo Bafna (Agarwal lab).

**Gordon Research Conference Computer Aided Drug Design**, West Dover VT, July 13-19, 2019; Rupesh Agarwal (Smith lab).

**Society for Molecular Biology and Evolution Conference**, Manchester, England, July 20-27, 2019; Alex Cope (Gilchrist lab).

**Computational Biophysics**, Pittsburgh, PA, May 12-18, 2019; Priyojit Das (McCord lab).

**Conference and Seminar on Multi-drug Efflux**, Lucca, Italy, April 26-May 4, 2019; Adam Green (Smith lab).

**American Association for Cancer Research**, Atlanta GA, March 30-April 4, 2019; Pawat Pattarawat (Wang lab).

**Gordon Research Conference Ecological and Evolutionary Genomics**, Manchester, NH, July 12-19, 2019; Katrina Schlum (Emrich lab).

**Gordon Research Conference on Mechanisms of Membrane Transport**, New London, NH,

June 21-29, 2019; Shantanu Shukla (Myles lab).

**Wind River Conference**, Estes Park, CO, June 5-9, 2019; Rachel Steele (Fozo lab).

**Gordon Research Conference Membrane Protein Folding**, Easton, MA, July 7-12, 2019; Katherine Stefanski (Barrera lab).

**70th Annual International Society of Electrochemistry Conference**, Durban, South Africa, July 29-August 11, 2019; Alex Teodor (Bruce lab).

**Southern Forest Tree Improvement Conference**, Lexington, KY, June 3-6, 2019; Jiali Yu (Staton lab).

## GRADUATIONS

**Suresh Poudel**, PhD 2018 (Hettich): Postdoc at ORNL, Hettich lab.

**Amanda (deVolk) Kennedy**, MS 2018 (Löffler).

**Grace (McSween) Satterfield**, MS 2018 (Morrell-Falvey): Science writing program, medical science writer.

**Prashasti**, PhD 2018 (Serpensu): Postdoc at Icahn School of Medicine, Mt Sinai, NY, Jian Jin lab.

**Sushmita Vijaya Kumar**, (Morrell-Falvey): PhD 2018: Postdoc at Scripps Institute of Oceanography, UC San Diego, La Jolla, CA, Brahamsha lab.

**Jennifer Bourn**, PhD 2018 (Cekanova): Postdoc at University Cincinnati, OH, Waltz lab.

**Ming Chen**, PhD 2018 (Staton): Data scientist at Cryoocyte, Inc; Atlanta, GA.



## BUILDING BRIDGES IN THE CITY OF BRIDGES

Last May, Priyojit Das (McCord lab) attended the Hands-on Workshop on Computational Biophysics at the Pittsburgh Super Computing Center (PSC). The objective of the workshop was to bridge the gap between the two major categories of biomolecular structural and functional study - normal mode analysis and molecular dynamics simulation - and how these categories can be used together to solve structural and dynamic relationships in proteins. Over the course of 5 days, the workshop covered a wide variety of physical models and computational techniques for the modeling and simulation of (mainly) proteins of different scales, using elastic network models (Gaussian network models and Anisotropic network models), ProDy (Protein Dynamics and Sequence Analysis), NAMD (Nanoscale Molecular Dynamics) and VMD (Visual Molecular Dynamics). The case studies included simulations of proteins in biomembranes, mechanisms of molecular motors, signaling pathways, druggability simulations, and ion channels.



View of the Carnegie Mellon campus (left) and the city of Pittsburgh from the Cathedral of Learning at the University of Pittsburgh.

Priyojit had only praise for the organizers: "Dr. Ivet Bahar and Dr. Emad Tajkhorshid each represent one of the major modeling strategies. Along with the PSC staff they did a wonderful job. The graduate students and postdocs from their labs met each participant individually to help them solve their own research problem. For example, Dr. Tajkhorshid and his postdocs gave me useful suggestions about my large scale coarse-grained genome simulation project."

Though most of the workshop was dedicated to hands-on tutorials, the organizers arranged a 10 minute research presentation for all attendees. "That gave me the opportunity to present my work on the characterization of biomolecule structure and dynamics using contact map analysis in the workshop. Dr. Ivet Ba-

har from the University of Pittsburgh is highly recognized for studying the structure and dynamics of biomolecules using elastic network models. Her group's work and my collaborator, Dr. Tongye Shen's work also match to some extent. It was gratifying to receive very positive feedback on my work from Dr. Bahar and her group."



Computational Biophysics workshop at the University of Pittsburgh. The organizers, Dr. Ivet Bahar and Dr. Emad Tajkhorshid, are seated in the second row, third and fourth from the left. Priyojit Das is in the third row, second from right.

At that time, PSC had just begun to invite proposals for the new Anton 2 supercomputer, one of the most powerful systems for molecular simulations. Anton (version #1) supported the work of prior GST students such as Xiaohu Hu (Smith lab) in the past. Priyojit: "It turns out that our coarse-grained chromosome system does not lend itself to be simulated on the Anton 2. However, I had the opportunity to discuss with the PSC's senior director of computational biology, Mr. Phil Blood, what other PSC resources can be used for my whole-genome simulation work."

Priyojit also carved out some time to explore the city of Pittsburgh and the university. "It is a beautiful place and its historical architecture can amaze any person. The 'Cathedral of Learning', 535 feet tall, is not easy to overlook, and a must-visit, as are the Carnegie Museum and Libraries on the neighboring Carnegie-Mellon campus."

Priyojit recommends attending high-end workshops such as this one as at least equally beneficial as any conference. "Besides learning new things, we get the opportunity to make new connections, and it is a refreshing break from daily life."

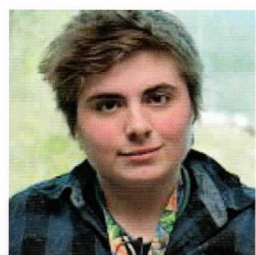
Link: <https://mmbios.pitt.edu/hands-on-workshop-on-computational-biophysics-2019>



## SNAPSHOTS OF STUDENTS' RESEARCH



**Gut wrenching.** A dynamic community of microbial organisms populates the gastrointestinal tract of humans, particularly in the colon. These microbes play an active role in the health of their host through assistance with digestion and immune modulation. In some cases, they are believed to cause autoimmune diseases. To date most techniques that study these microbes are pretty good at identifying them, but less good at showing what they are doing. Metaproteomics is a promising up and coming technique that measures the protein complement of a microbial community directly from the environmental sample. In this study, Alfredo Blakeley-Ruiz and coworkers from the Hettich lab explored whether patients suffering from Crohn's disease shared a similar microbial protein complement. The answer was that the microbiome proteomes varied substantially between patients and over time. However, the specific functions represented by these proteins were fairly similar across samples and were observed across multiple distant microbial lineages. This implies that specific biochemical functions rather than the species identities of the microbes might be a better place to explore gut microbiomes associated with disease. This work was published in the journal *Microbiome*.



**Bacterial bouncers.** Bacteria are developing resistance mechanisms to antibiotic treatments at an alarming rate and resistance has been detected against every approved antibiotic on the market. Overcoming antibiotic resistance in Gram-negative bacteria is challenging due to synergistic interactions between the low permeability of the outer membrane and active multidrug efflux pumps. To separate these two barriers, the lab of Dr. Helen Zgurskaya at the University of Oklahoma developed strains of *Escherichia coli* and *Pseudomonas aeruginosa* that have hyperporinated outer membranes, lack efflux pumps, or both. GST student Sarah Cooper (Parks Lab) and colleagues used machine learning to compare computed physicochemical properties and experimentally measured activity data. From this analysis, they identified the most important properties that correlate with antibiotic activity. The identified properties obtained from this work provide a set of "rules" or guidelines that can be used for development and optimization of future antibiotics. This work was published in *ACS Infectious Diseases*.

## SELECTED RECENT PUBLICATIONS BY GST STUDENTS

**Cope AL, Hettich RL, Gilchrist MA.** (2018) Quantifying codon usage in signal peptides: Gene expression and amino acid usage explain apparent selection for inefficient codons. *Biochim Biophys Acta Biomembr.* 1860:2479-2485.

**Cooper SJ, Krishnamoorthy G, Wolloscheck D, Walker JK, Rybenkov VV, Parks JM, Zgurskaya HI.** (2018) Molecular Properties That Define the Activities of Antibiotics in *Escherichia coli* and *Pseudomonas aeruginosa*. *ACS Infect Dis* 4:1223-1234.

**Shukla S, Bafna K, Gullett C, Myles DA, Agarwal PK, Cuneo MJ.** (2018) Differential Substrate Recognition by Maltose Binding Proteins Influenced by Structure and Dynamics. *Biochemistry* 57:5864-5876.

**Kumar P, Selvaraj B, Serpersu EH, Cuneo MJ.** (2018) Encoding of Promiscuity in an Aminoglycoside Acetyltransferase. *J Med Chem.* 61:10218-10227.

**Varanasi SK, Rouse BT.** (2018) How host metabolism impacts on virus pathogenesis. *Curr Opin Virol.* 28:37-42.

**Lindsay RJ, Pham B, Shen T, McCord RP** (2018) Characterizing the 3D structure and dynamics of chromosomes and proteins in a common contact matrix framework. *Nucleic Acids Res* 46:8143-8152.

**Qian C, Chen H, Johs A, Lu X, An J, Pierce EM, Parks JM, Elias DA, Hettich RL, Gu B.** (2018) Quantitative Proteomic Analysis of Biological Processes and Responses of the Bacterium *Desulfovibrio desulfuricans* ND132 upon Deletion of Its Mercury Methylation Genes.. *Proteomics* 18:e1700479

**Johnson QR, Lindsay RJ, Shen T.** (2018) CAMERRA: An analysis tool for the computation of conformational dynamics by evaluating residue-residue associations. *J Comput Chem.* 39:1568-1578.

**Kapoor K, Cashman DJ, Nientimp L, Bruce BD, Baudry J.** (2018) Binding Mechanisms of Electron Transport Proteins with Cyanobacterial Photosystem I: An Integrated Computational and Experimental Model. *J Phys Chem B.* 122:1026-1036.

**Villalobos Solis MI, Giannone RJ, Hettich RL, Abraham PE.** (2019) Exploiting the Dynamic Relationship between Peptide Separation Quality and Peptide Coisolation in a Multiple-Peptide Matches-per-Spectrum Approach Offers a Strategy To Optimize Bottom-Up Proteomics Throughput and Depth. *Anal Chem.* 91:7273-7279.

**Blakeley-Ruiz JA, Erickson AR, Cantarel BL, Xiong W, Adams R, Jansson JK, Fraser CM, Hettich RL.** (2019) Metaproteomics reveals persistent and phylum-redundant metabolic functional stability in adult human gut microbiomes of Crohn's remission patients despite temporal variations in microbial taxa, genomes, and proteomes. *Microbiome* 7:18.

**Jia Q, Chen X, Köllner TG, Rinkel J, Fu J, Labbé J, Xiong W, Dickschat JS, Gershenson J, Chen F.** (2019) Terpene Synthase Genes Originated from Bacteria through Horizontal Gene Transfer Contribute to Terpeneoid Diversity in Fungi. *Sci Rep.* 9:9223.



# WELCOME, CLASS OF 2019!



## Manasa Appidi

graduated with a master's degree in Biology from Long Island University, Brooklyn, NY. She was awarded "Top Graduate Scholar" for the year 2016 in recognition of outstanding academic achievement. Prior to this, she also earned a MS degree in Biomedical Basis of Disease from Sheffield Hallam University, UK. She gained research experience in microbiology and molecular biology techniques. She is currently working in a pharmaceutical testing laboratory, widely

using analytical instrumentation. She is interested in the fields of proteomics and computational biology.

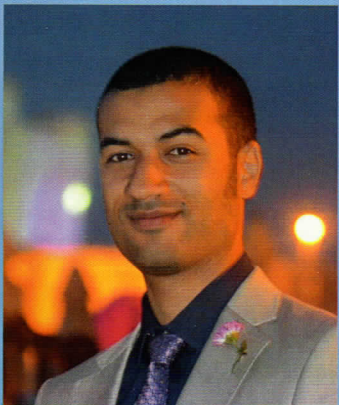
## Barbra Dompseh

graduated with a BS in Biochemistry, Cell and Molecular Biology from the University of Ghana in 2017. She has participated in various undergraduate and postgraduate internship opportunities, with one being at the Noguchi Memorial Institute for Medical Research (NMIMR) where she aided efforts in research on chronic kidney disease in individuals of African and African-American origin. Currently, working on oncoviruses she has garnered significant research experience in microbiology and molecular biology. Her keen interest in human genetics led her to apply to the GST program at UTK.



## Ahmed Elshaarawi

earned his first degree in Zoology at the University of Alexandria in Egypt. He then attended the University of North Carolina Greensboro on a Fulbright Fellowship and completed a Master's Degree in molecular and cellular biology. He joined GST in January 2019. Ahmed is interested in the molecular basis of human disease including cancer. He comes with some hands-on experience in computational biology and Python programming and is eager to expand his expertise in bioinformatics.



## Ziyi Liu

graduated with a BS degree from Southern University of Science and Technology. She already spent a semester working in the computational modeling group of Dr. Tian Hong. She is interested in mechanics of processes in biological systems, for example, the dynamic connection among different biological systems and reactions of these systems to the environment. In addition, she likes painting very much.

## Cole Sawyer

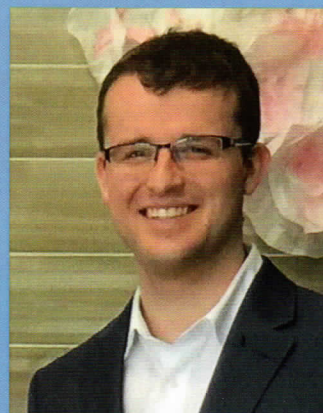
graduated from the South Dakota School of Mines and Technology with a bachelor's degree in Applied Biological Sciences. He currently works at the Oak Ridge National Lab as a research assistant in the labs of Jessy Labbé and David Graham. Both of his projects center around the CRISPR/Cas9 system as it pertains to biosecurity, specifically the prevention and detection of unwanted gene editing events. He looks forward to continuing this work into graduate school.



**Steven Tavis** graduated with a BS degree in Biology from Truman State University in Kirkwood, MO. He conducted extensive research over the summers, with Dr. Alessandro Vindigni at St. Louis University on genotoxic stress and DNA repair, and for three summers in the lab of Dr. Jennifer Lodge at Washington University in St. Louis. In the Lodge lab he was involved in research to generate vaccines against an opportunistic fungal pathogen of humans. Thus, he is curious about solutions to both fundamental and applied questions in molecular and cellular biology. He has experience in customizing the computational analysis of experimental data and is interested in the application of bioinformatics tools to biomedical questions.

## Andrew Willems

graduated with a BS degree in Biology at UT Knoxville. His interests mainly center on using computational tools and techniques to answer biological questions. In particular, he hopes to pursue research focused on using approaches that involve the use of big data, deep neural networks, and mathematical models to better understand the formation and progression of human disease. Andrew has research experience in microbial genomics from the lab of Dr. Sarah Lebeis.



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