STRUCTURES

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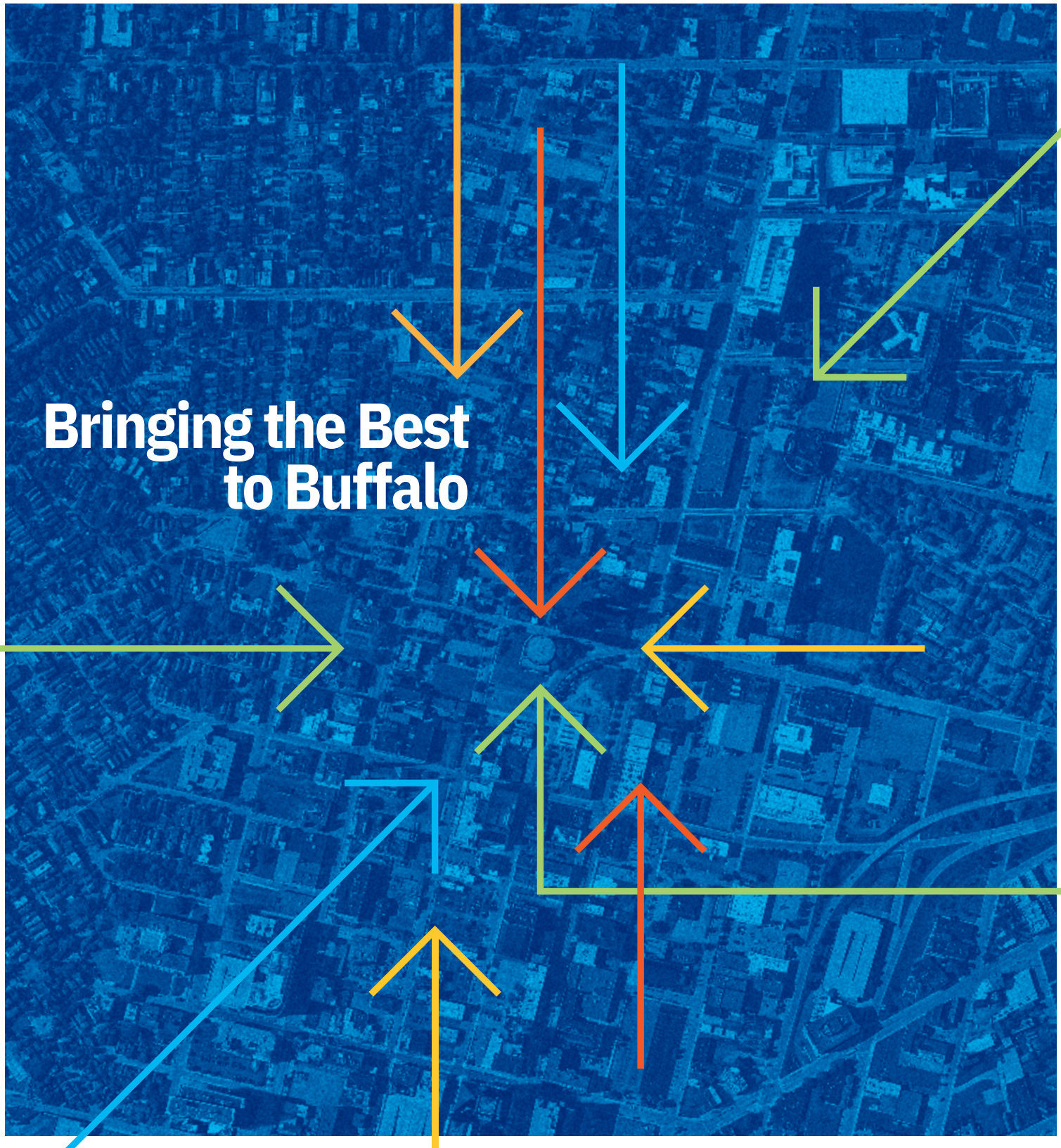


Bringing the Best to Buffalo

We are proud of the diverse team

we are building at the Institute.

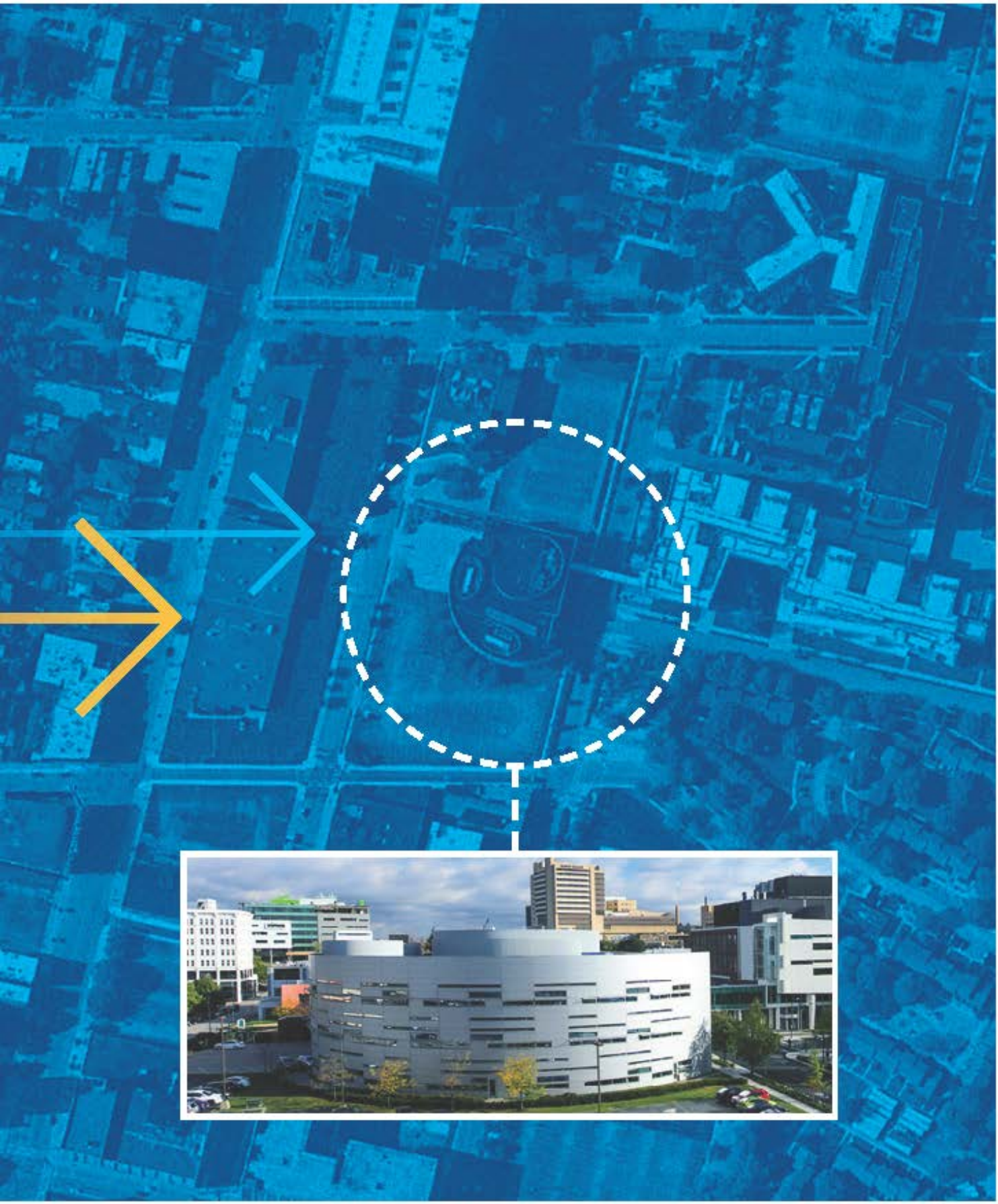
We have several new PhD scientists

working in our laboratories,

some who have returned to Buffalo

and some who are calling Buffalo their home

for the first time.



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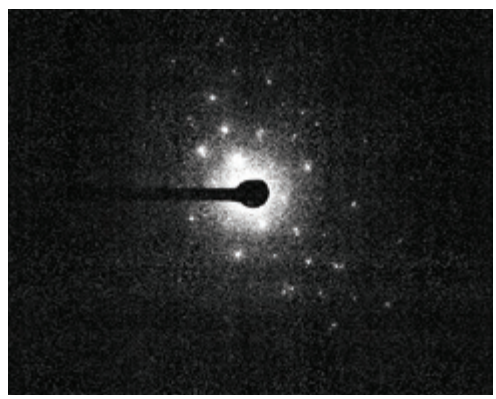

SEVEN QUESTIONS | 35

You too can make an impact in a multitude of ways and create your own legacy.

STRUCTURES

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A MESSAGE FROM THE CSO

The theme of this year's edition of Structures is 'Bringing the Best to Buffalo.' There have been a lot of changes at the Institute with new faces and new opportunities for some of those faces already here. There have been new scientific results and collaborations worldwide that have enabled these discoveries. There have been events to help raise awareness of what we do at HWI and support our mission. A lot has happened since our last issue.

EDWARD SNELL, PhD
Chief Scientific Officer
Hauptman-Woodward
Medical Research Institute

We are proud of the diverse team we are building at the Institute. We have several new PhD scientists working in our laboratories, some who have returned to Buffalo and some who are calling Buffalo their home for the first time. We have new technicians and new members of our administrative team and you will read more about them here. We are recruiting two new scientific teams and we'll talk about them in the next issue—it is an exciting time at our organization and we are thrilled to have you join us on this journey.

Our Cryo-Electron Microscopy (Cryo-EM) Center is generating results and working with a mixture of academics and industry. We want to ramp up the operational tempo and accelerate research into cures and treatments for existing diseases, and understanding new ones. The Center allows us to continue to be state-of-the-art in the field and is helping us attract our new scientific teams.

Internally, there is a synergy between the Cryo-EM Center and the National Crystallization Center. We are harnessing that synergy in the Institute's tradition of developing new technology to aid the whole field. Our scientific impact continues, and our team in Chicago played a small but critical part in enabling the development of Paxlovid,™ detailed in this issue.

We are growing our strategic goals and initiatives in education, currently with the interns we work with over the summer and as part of our National Science Foundation-supported BioXFEL Center. Excitingly, one of the interns from the BioXFEL program, an undergraduate student, won the top poster prize at the annual LCLS/SSRL users meeting, a premier X-ray user facility in the USA, beating graduate students and postdoctoral fellows. We are working to develop a new educational opportunity targeting underserved communities in the region, and one of our postdoctoral fellows has been accepted for a prestigious fellowship with the National Institutes of Health. HWI is educating future scientific leaders at every level, encouraging them along their professional journeys.

There is also a personal journey. After nine years of leading the Institute as CEO (and scientific researcher) I have stepped aside to fill the role of Chief Scientific Officer. Our Board of Directors is conducting a national search and investing in a full-time CEO to continue the growth and impact of HWI. It's an exciting time for the future of the Institute and I hope you will see that as you read on and follow us on our social media channels.

For those who have supported us, thank you, we really appreciate what you enable us to do and contribute to medical research worldwide. For those who would like to make a difference, please consider supporting our mission, and join us on our journey, leading to new discoveries.

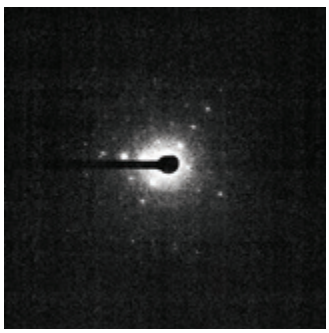
Seeing the Invisible

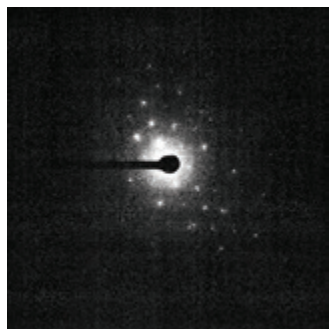
We've been talking a lot about cryogenic electron microscopy in past editions of the magazine. It's cool in all uses of the word. One of the most essential and fundamental requirements for understanding disease and how to develop drugs for treatment is the ability to image the biomolecules that can cause disease. Recent technological breakthroughs in cryogenic electron microscopy (cryo-EM) are revolutionizing this process and we now have this capability. Cryo-EM has become a powerful way to see the otherwise invisible structures of biological macromolecules. Application of this breakthrough technology has already allowed observation of drug-protein complexes which play central roles in neurology, cardiovascular diseases, and oncology. The Hauptman-Woodward Institute (HWI) is investing in this technological innovation with the establishment of the Cryo-EM Center.

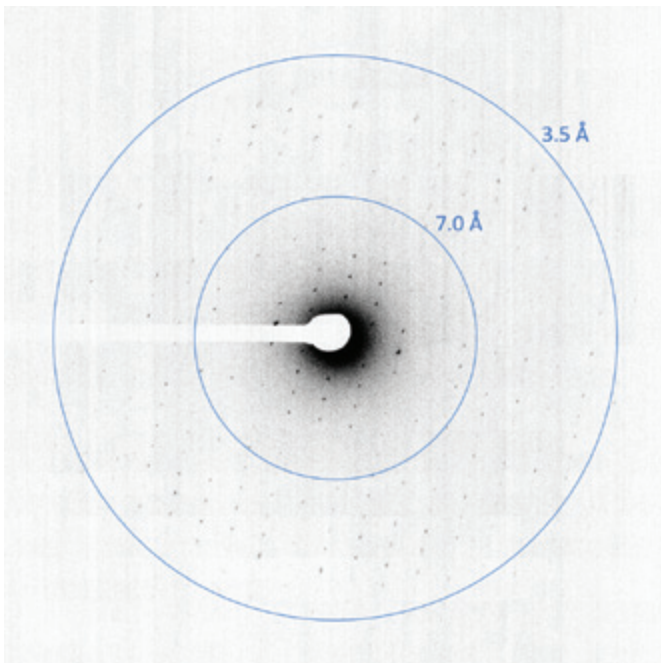
The new Cryo-EM Center helps research at HWI because it accelerates the structural determination of macromolecules and their complexes. The microscope's high throughput, enabled by fast detectors and improved imaging techniques, also makes it possible to offer equipment and services to academic and industry research groups expanding the impact of the Institute and putting Buffalo on the map. The Center is already working with Institute scientists, other academics in New York State and beyond, and some major industry names. It is a first step for the Institute in this growing technological area and we will grow our activities.

The Center is directed by Dr. Devrim Acehan who began his journey in structure-function relations of the biological molecules during his undergraduate studies in Bilkent University in Turkey, and worked on theoretical models and computer simulations. During his graduate studies at Boston University, Devrim obtained the first 3-D model of an apoptosome complex using single-particle cryo-EM methods, an important element in many diseases such as neurodegeneration and cancer. As a postdoctoral fellow at New York University (NYU), he developed and applied electron microscope tomography methods to study desmosomes, found in tissue that experiences intense mechanical stress such as cardiac muscle in the heart. As a junior faculty member at New York University he started studying structural effects of cardiolipin depletion, important in understanding how to treat heart disease, using cryo-electron tomography methods. Later, in electron microscopy core facilities at European Molecular Biology Laboratories, the Rockefeller University and the Weill-Cornell Medical College, he had the opportunity to work on diverse projects with scientists across the globe. Dr. Acehan was attracted to Buffalo by HWI and was excited to join as the director of the Cryo-EM Center.

Dr. Katherine Spoth joins HWI as a cryo-electron microscopist who came to us from Cornell University where she received her PhD in applied physics studying novel imaging techniques in cryo-EM. She went on to a research staff position supporting the operations







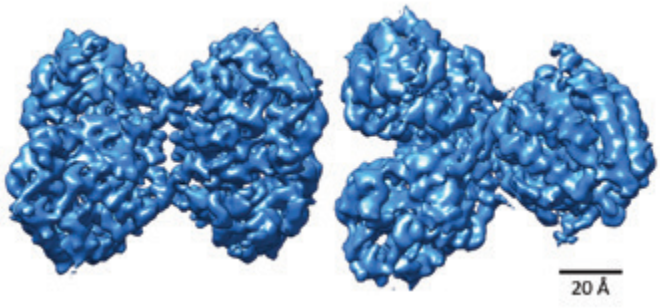
Merging the two-plus decades of crystallographic expertise with HWI's Cryo-EM Center to develop new methods.

of Cornell's first dedicated cryo-transmission electron microscope. Katie is a Buffalo native and earned her Bachelor's in physics and mathematics from the University at Buffalo. "It's so impactful to have cryo-EM in Buffalo, and I'm so grateful for the opportunity to do this work in my hometown." Her favorite part of working in a facility is the opportunity to work on many diverse projects and meet the scientists leading them, learning something new every day.

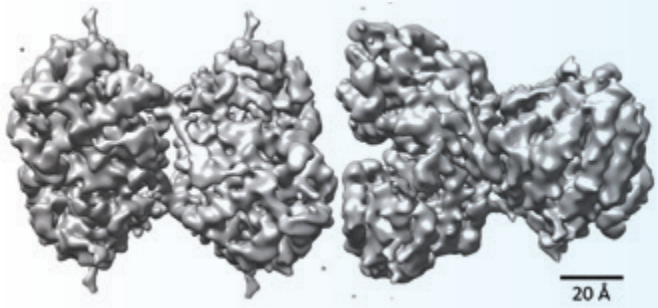
Combined, their experience with different techniques in cryo-electron microscopy, allows them to develop project-specific workflows to achieve the highest possible resolution that the new generation microscopes and direct electron detectors can provide. Together they are working on new imaging and data analysis techniques to improve results for challenging specimens. In collaboration with scientists at the Institute, they are developing methods to prepare and detect small crystals for electron diffraction experiments and obtaining 3-dimensional protein molecule models.

Outside of the Institute, The Cryo-EM Center has successfully worked closely with multiple academic groups and industry partners, developing ongoing relationships with many. Internally, two samples from Dr. Diana Monteiro were analyzed to provide structural detail at 3.4 Å resolution, a thousand times smaller than a regular microscope can even see. The protein has a complicated name, 3-Deoxy-D-arabinoheptulosonate 7-phosphate (DAHP) synthase (also known as Aro3), an essential enzyme for the survival of many microorganisms. The enzyme is involved in the production of amino acids such as phenylalanine and tyrosine. Humans cannot produce these amino acids themselves and do not have such an enzyme. This fact makes Aro3 a potential new drug target of special interest to fight fungal infections, a rising threat in the US.

The specific version of Aro3 that Dr. Monteiro works with comes from a newly emerged fungus, Candida Auris, which is considered an urgent threat by the Centers of Disease Control as it can cause bloodstream infections that kill 60% of patients. Antifungal drugs are severely underdeveloped, with the last new class of drugs developed more than two decades ago. Fungi and humans are genetically rather similar, limiting the number of proteins that can be targeted for therapies that do not cause severe side effects. The study of fungal enzymes and the understanding of their mechanisms and dynamics is vital for the improvement of therapies to combat such devastating fungal diseases, especially in those with weakened immune systems such as cancer and organ transplant patients, or anyone with immune system diseases. An image of Aro3 taken with our new microscope is shown.



Two samples from Diana Monteiro were analyzed to provide models at 3.4 Angstrom resolution. Holo (blue) and apo (gray) forms of Aro3 enzyme involved in the biosynthesis of aromatic amino-acids and a potential anti-fungal target that shows allosteric dynamics.



For scale, an Angstrom (Å) is 0.1 nm, or 100,000 times smaller than the width of a human hair.

To the expert eye one can see the structural components that make up the protein and start to obtain an understanding of how it works, much like a mechanic opening the hood of a car, seeing the engine, and understanding how the parts of that engine make the car run.

Disease is caused by the proteins (the basic biological machinery) in our body and Cryo-EM allows us to see those machines directly. These proteins are very small, smaller even than color. Cryo-EM uses electrons instead of light to image these proteins and can directly provide a three-dimensional image. The other technique available to us, X-ray crystallography, requires us to grow a crystal of the protein, a process we are very good at, but even so, one that fails more often than it succeeds. Cryo-EM increases our success rate in making the invisible visible, but it, too, has limitations. We can see the larger machines, viruses, complexes of proteins interacting etc. but are limited when those proteins that cause disease are too small.

To overcome this, we can access another method, micro electron diffraction, that the Cryo-EM Center brings to us. Sometimes crystals can be grown, but they are too small for X-ray diffraction. Electrons can be diffracted and the Cryo-EM Center is working closely with the National Crystallization Center on diffraction with electrons, a process which can overcome the size limit of Cryo-EM, and may help in the difficulty of growing some crystals for X-ray crystallography. This is a growing research area and Drs. Sarah Bowman and Miranda Lynch from the National Crystallization Center have been awarded a $1.5M grant by the National Institutes of Health to develop tools to detect and handle nanocrystals for cutting edge structural biology methods. This builds on the expertise and capabilities of both the National Crystallization and Cryo-EM Centers.

National High-Throughput Crystallization Center

Structural biology is the study of the architecture of biological molecules. The three-dimensional maps of the molecules that we get when we determine their structures help us to figure out how they work: how they function when we are healthy and what changes happen when we are diseased. By understanding structures, we can better understand both the diseases and molecules that can be designed to treat and cure disease. Close to 90% of these structural models have been determined using the structural biology technique X-ray crystallography. To get a crystal structure, first you need a crystal. This is one of the most challenging steps in the structure determination process; overcoming this primary bottleneck is what we focus on in the National High-Throughput Crystallization (HTX) Center at HWI.

The HTX Center works with a thriving worldwide structural biology research community and has been in operation in Buffalo, NY for over two decades. In 2021, we received funding from the National Institutes of Health (NIH) designating the HTX Center as a National Resource. Scientists from around the world send samples to HWI for the unique crystallization experiments and imaging that we provide. The HTX Center provides access to a centralized facility for crystallization expertise, training, and instrumentation not typically available at independent laboratories; we facilitate efficient and cost-effective crystallization of biological macromolecules for academic, non-profit, government, and industry users.

The critical role of X-ray crystallography in structural studies was observed in real-time as the COVID-19 pandemic unfolded. Crystal-based structures informed on key steps in the development of vaccines and treatment against the disease. The HTX Center has been an important contributor to the research on COVID-19. We were contacted early in the pandemic for help with crystallizing many of the proteins that make up SARS-CoV-2, the virus that causes COVID-19. Since then, we have successfully assisted multiple research groups in the fight against the pandemic, with additional funding from both the National Science Foundation and the National Institutes of Health supporting these efforts. Importantly, many of the crystallization experiments at the HTX Center involved screening potential drugs designed to target the virus. Additionally, in the past several years the HTX Center has supported work developing therapeutics for cancer treatments (for squamous cell carcinoma, acute lymphoblastic leukemia, and breast cancer), novel antibiotics, and research on bacterial and fungal pathogens.

The HTX Center has a vibrant presence in the structural biology community. As we grow, our team of experts is stepping up to develop new pipelines, to work with an expanding base of new users, and to take on new challenges.

To learn more about the National Crystallization Center, visit **getacrystal.org.**

Elizabeth Snell

Dr. Miranda L. Lynch

Tiffany R. Wright

Dr. Sarah EJ Bowman

Dr. Gabrielle R. Budziszewski

THE HTX CENTER TEAM

DR. SARAH EJ BOWMAN is the HTX Center Director and an Associate Investigator at HWI. She has been working in structural biology for over 15 years. She completed her PhD in Chemistry with Professor Kara Bren at the University of Rochester. Dr. Bowman then moved to the Massachusetts Institute of Technology for postdoctoral research with Professors Catherine Drennan and Collin Stultz (supported by an NIH Ruth L. Kirschstein NRSA fellowship), followed by a second postdoctoral appointment at Los Alamos National Laboratory. Dr. Bowman joined HWI as the Director of the Crystallization Center in July 2017. Her research group at HWI is working to combine crystallographic and spectroscopic approaches to answer fundamental questions about protein biochemistry, especially in metalloproteins, as well as developing new methods for crystallization of biomolecules and detection of nanocrystals.

DR. MIRANDA L LYNCH is an Assistant Investigator at HWI, having joined the Institute as a Staff Scientist in 2018. She is a quantitative and computational scientist focused on applications in structural biology and image analysis. She received her PhD in Statistics from University of Rochester on Bayesian methodology, and continued to a postdoctoral fellowship at Harvard TH Chan School of Public Health on modeling methods for HIV disease progression. Her work in the HTX Center focuses on imaging and computational aspects of the crystallization pipeline. Her research has a focus on how we can use imaging methods to better detect and characterize samples for structural biology techniques. In addition to developing quantitative methods to make better use of imaging for crystal growth and detection, she also pursues computational approaches for understanding protein motion from structural data.

DR. GABRIELLE R BUDZISZEWSKI is the HTX Center Operations Manager and joined HWI in Fall 2022. She is a native Buffalonian who completed her bachelor's in biochemistry at Canisius College prior to moving to the University of North Carolina at Chapel Hill for her PhD in Biochemistry & Biophysics working in Rob McGinty's Lab. She has expertise in macromolecular crystallography, recombinant protein expression and purification, enzymology, and biochemical assay development. Dr. Budziszewski is passionate about working with users to develop strategies to produce diffraction-quality crystal hits and promoting an inclusive scientific work environment.

ELIZABETH SNELL is a Research Associate in the HTX Center and joined the team in March 2022. She received her B.S. in Chemistry from the University of Alabama in Huntsville. She worked in industry for several years, focusing on protein PEGylation. She has more than 15 years of experience in protein crystallization. Several of the proteins that she has crystallized have flown on the International Space Station. She is currently working on best ways to optimize crystallization results for HTX Center users and on developing ways to tune crystal growth size for specific experiments.

TIFFANY WRIGHT is a Research Associate in the HTX Center, starting in November 2022. New to the area of structural biology, she brings her experience to the lab from her background as a B.S. in Forensic Chemistry from Buffalo State College. Her work focuses on high-throughput protein crystallization, and she maintains daily operations and service output in the HTX Center.

New faces at IMCA

Pictured from left to right, are Dr. Lisa Keefe, Dr. John Bacik, Dr. Erica Duguid, J. Lewis Muir, Davis Dunn, and Bruce Lawson.

The Advanced Photon Source at the Argonne National Laboratory (image provided by Argonne National Laboratory).

THE HAUPTMAN-WOODWARD MEDICAL RESEARCH INSTITUTE OPERATES A BEAMLINE FACILITY HEADED BY DR. LISA KEEFE, for eight pharmaceutical companies, AbbVie, Bristol Myers Squibb, Evotec, Janssen, Merck, Novartis, Pfizer, and Relay Therapeutics. It also supports numerous smaller companies that make use of the expertise and facilities to develop new pharmaceuticals and help the economy of the nation. The beamline is called the Industrial Macromolecular Crystallography Association Collaborative Access Team.

The beamline is situated at a Department of Energy Facility called the Advanced Photon Source at the Argonne National Laboratory, just west of Chicago. The facility is undergoing a massive upgrade process and when this is finished the X-rays will be the most brilliant in the world, and the beamline one of the best.

Three new staff have joined the beamline since our last issue of Structures. They are Dr. John Bacik, Davis Dunn and Bruce Lawson.

John is a Cornell-trained crystallographer who works closely with many of the largest pharmaceutical companies at the beamline at the Advanced Photon Source in Chicago. This facility, the Industrial-Macromolecular Crystallization Association Collaborative Access Team (IMCA-CAT) looks at hundreds of potential new drugs every day and is the world's premier structural biology facility for the pharmaceutical industry. Dr. Bacik joins the team there to help with this process.

Davis joined as a Research Engineer. He has a Bachelor's in Chemical Engineering from Purdue University and experience as a field service engineer for industry.

Bruce joined as a Research Beamline Technician and was a graduate of Dr. Jason Benedict's laboratory at the University at Buffalo and has a Chemistry degree. In this case, his journey was not to Buffalo, but from Buffalo to join our group running the beamline.

The IMCA-CAT team saw a significant changeover during the COVID-19 pandemic. The staff in place now are utilizing synchrotron sources worldwide during the upgrade of the Chicago facility. They will be bringing the best ideas back to IMCA-CAT for when the facility reopens in 2024.

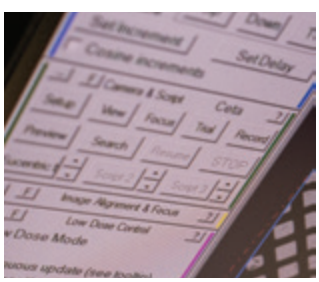
Structural Biology at HWI

The Hauptman-Woodward Medical Research Institute has a rich history in the field of structural biology, contributing to the world's knowledge of how biological mechanisms function, how disease occurs, and how drugs can be developed to treat disease. Part of this process has been developing the tools to makes this happen and providing those tools for the community to use.

For over 20 years, we have helped the international scientific community to obtain crystals of the biological components that drive disease. Almost 20,000 proteins later and we were named the National Crystallization Center by the National Institutes of Health—recognizing our role in the field.

While the Institute has offered crystallization services to academic users through the Crystallization Center and later managed a facility at the Advanced Photon Source at the Argonne National Laboratory near Chicago, HWI is now formally making its expertise available to all, and collectively offering a complete set of structural biology solutions on a fee-for-service basis.

We offer accessible Cryo-EM, comprehensive crystallization services, and streamlined synchrotron X-ray data collection to both academic and industrial clients providing industry-level capabilities at the highest standards for quality, reliability, efficiency, and productivity while providing confidentiality and expert support for challenging experiments. We are invested in your success by providing cost-effective access to world-class research capabilities.



The services team leadership consists of Dr. Devrim Acehan, Director, The HWI Cryo-EM Center, Dr. Sarah Bowman, Director, National High-throughput Crystallization Center, Dr. Lisa Keefe, Executive Director & VP for Advancing Therapeutics, IMCA-CAT, who together with their teams provide many years of expertise in structural biology solutions. Our services are collectively known as Structural Biology Solutions at HWI and are supported with a new website: **structuralbiologyservices.com**.

What Can You Expect from Structural Biology Services at HWI?

EXPERTISE & CONFIDENTIALITY

- Decades of combined technical expertise & scientific knowledge to help you develop project strategies
- Serving academic and proprietary users confidentially for over two decades

STATE-OF-THE-ART INSTRUMENTATION

- Timely access to instrumentation that is otherwise cost-prohibitive for individual researchers
- Rapid data delivery to keep your projects on track

INNOVATION

Timely access to instrumentation that is otherwise cost-prohibitive for individual researchers

Rapid data delivery to keep your projects on track.

Since the Structural Biology Services group was started, the Institute has worked with many academic groups and industrial partners. The Services group provides our expertise to promote overall progress in structural biology and leverage efforts to develop new cures and treatments, while aiming to generate resources that can be reinvested in the Institute To learn more about HWI's Research Services, visit **hwi.buffalo.edu/research-services.**

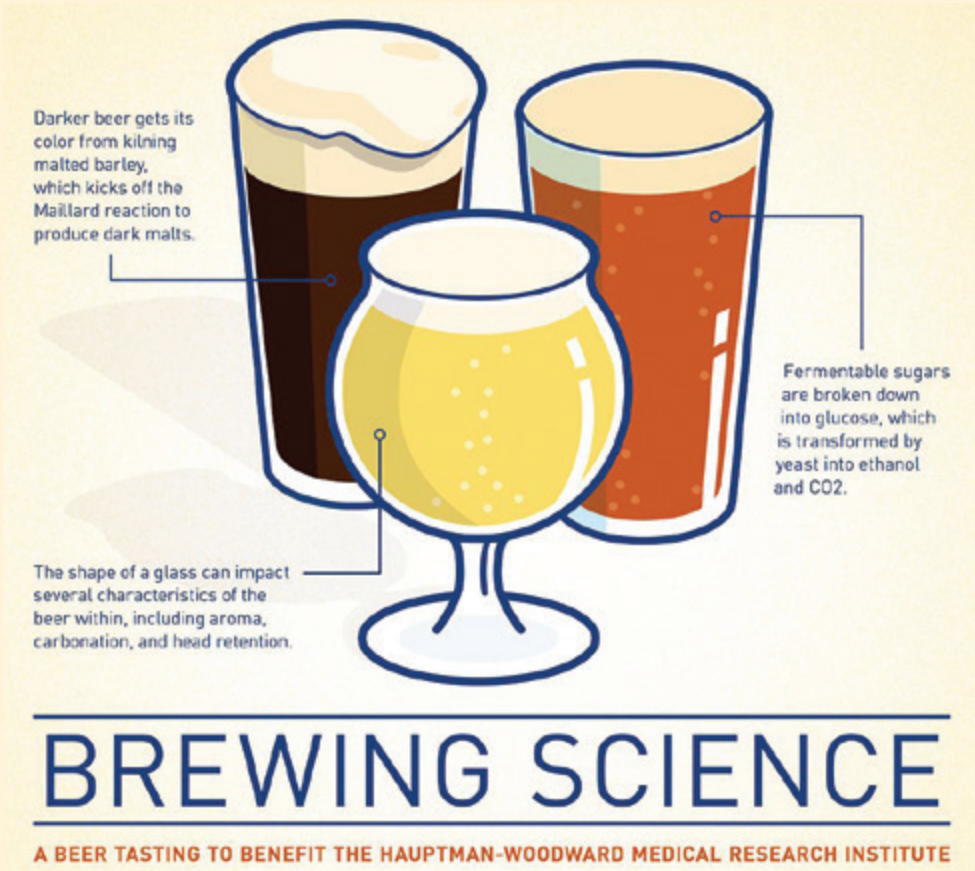
William Harries and Sean Moskal bring depth to the HWI Board

Dr. William Harries is the chief scientist at Aromyx Corporation and is an accomplished protein biochemist, structural biologist, and cell biologist with over 20 years of laboratory research experience in high-throughput recombinant membrane protein expression, protein design, protein purification, protein crystallization, and structure determination.

Dr. Harries has personnel management experience in a large academic laboratory environment and working with pharmaceutical, biotech companies, a wide variety of academic institutions and government organizations.

Sean Moskal is the Senior Vice President, at Key Bank in Buffalo, New York. He is an experienced Corporate Banker with International experience and a consistent track record of delivering growth through both deepening customer relationships and new client acquisition. Sean is another person whose journey has brought him back to Buffalo after spending 12 years at HSBC with stops in Chicago and Hong Kong.

HWI kicked off Summer 2023 with its annual BREWING SCIENCE event held on June 22. The BNMC Pocket Park once again served as the perfect venue for our guests to sample beer from several local breweries, enjoy delicious food from Osteria 166, and play lawn games accompanied with music by DJ Eric. Many thanks to our generous sponsors and our dynamic and dedicated 2023 class of HWI Young Professionals who made this event possible. Please stay tuned for more information about our 2024 Brewing Science event!



CELEBRATING INNOVATION AT unGALA 2023

ON OCTOBER 27, THE INSTITUTE WELCOMED FRIENDS AND COMMUNITY PARTNERS TO THE UNGALA, its major fundraising event of the year. This year's event took place in the Forbes Theatre at 500 Pearl. Event co-chairs Dan and Stephanie Magnuszewski highlighted the many reasons to celebrate HWI, the crucial work they have accomplished throughout the years and all that there is to look forward to in the future of our Institution.

The "fabulous casual" event featured bourbon tasting provided by Brighton Wine and Liquor, samples of rasta pasta from Chef Darian Bryan, chocolate and desserts by Jannell Easton of Nikki's Chocolates, wine tasting by Robert Renzoni Vineyards, and chocolate pairing by Dark Forest Chocolate.

Many thanks to the generosity of our sponsors and all those who were in attendance to celebrate innovation and reconnect with friends, old and new.

OUR 2023 HONOREES

HELEN WOODWARD RIVAS AWARD

Recognizes a person who has made major contributions to the Institution through long and distinguished service.

Jane F. Griffin, PhD

DR. GEORGE F. KOEPF AWARD

Recognizes a person who has made major contributions to the intersection of scientific research and clinical applications, and is a friend of the Hauptman-Woodward Institute.

Thomas A. Russo, MD

OUTSTANDING SERVICE AWARD

Recognizes exceptional leadership that enabled HWI to realize a collective vision in our state-of-the-art research facility.

John G. Horn, Esq.

ALLISON JENSEN YOUNG PROFESSIONAL AWARD

Recognizing participation in and contributions to HWI through the Young Leadership program.

Ryan Sheehan, CIC, AAI

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BOURBON TASTING PROVIDED BY

Brighton

Drs. Edward Snell and Stephan Ginell elected to Fellow of the American Crystallographic Association—the Structural Science Society.

The American Crystallographic Association—the Structural Science Society—established the Fellows distinction to recognize a high level of excellence in scientific research, teaching, and professional duties, but also service, leadership, and personal engagement in the world of crystallography and science. The Fellows distinction celebrates the excellence of American Crystallographic Association members and promotes their recognition worldwide to constituencies outside, such as their employers, other scientific societies, and the government. Fellows serve as scientific ambassadors to the broader scientific community and the general public to advance science education, research, knowledge, interaction, and collaboration.

Drs. Edward Snell (Chief Scientific Officer of the Hauptman Woodward Medical Research Institute) and Stephan Ginell, an adjunct member of the Institute and scientist with the Industrial Macromolecular Crystallography Association beamline in Chicago (operated by the Institute) were elected fellows of the American Crystallographic Association—The Structural Science Society. Six fellows were named in 2022 and HWI is proud that two of those are from its scientific staff. Drs. Snell and Ginell join Dr. Lisa Keefe, Executive Director of the Industrial Macromolecular Crystallography Association beamline, as Fellows associated with the Institute in Buffalo.

A Fellow is defined as "a Member whose efforts on behalf of the advancement of crystallography or its applications that are scientifically or socially distinguished." Examples of areas in which nominees may have made significant contributions are research; teaching; technology; services to professional societies; administration in academia, industry, and government; and communicating and interpreting science to the public. Fellows are elected annually by the current group of Fellows.

Drs. Snell and Ginell are proud to be joining the ACA Fellow ranks, which include three Nobel laureates. Dr. Snell was "both humbled and honored by this recognition", and Dr. Ginell noted that "he was surprised and also honored." Previously elected Fellow Dr. Lisa Keefe said "It is an honor to welcome Drs. Snell and Ginell as ACA Fellows. As engaging and active members of the ACA for many years, they are exemplary scientists and mentors, visionary leaders, and strong champions of crystallography and structural science." It demonstrates the impact of structural biology in Buffalo and its recognition nationally.

PAXL

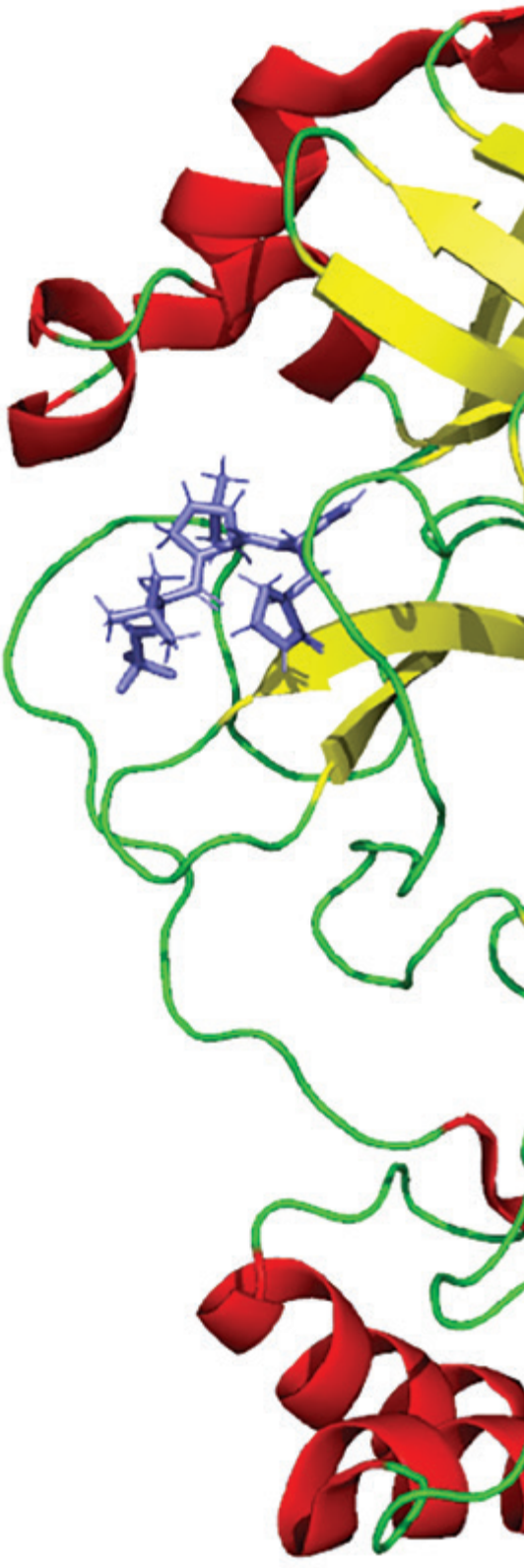
MAKING IT HAPPEN

VID

PAXLOVID IS AN ANTIVIRAL PILL FOR COVID-19 that can be taken at home to help keep high-risk patients from getting so sick that they need to be hospitalized. The drug, developed by Pfizer, had an 89% reduction in the risk of hospitalization and death in unvaccinated people. Studies have since confirmed Paxlovid's effectiveness among people who have been vaccinated. Paxlovid consists of two separate medications packaged together. When you take your three-pill dose, two of those pills will be nirmatrelvir, which inhibits a key enzyme that the COVID virus requires in order to make functional virus particles. After nirmatrelvir treatment, the COVID virus that is released from the cells is no longer able to enter uninfected cells in the body, which, in turn, stops the infection. The other is ritonavir, a drug that was once used to treat HIV/AIDS but is now used to boost levels of antiviral medicines.

A critical component of the COVID-19 virus is a protein called the main protease which takes the material the virus produces in the body and cleaves it into individual components allowing the infection to proceed. This viral protease has a unique feature not seen in human proteases that offered selectivity to target the viral material. An enormous amount of work took place by Pfizer to identify potential pharmaceutical leads that targeted this protease. Those leads demonstrated significant potential and structural biology techniques were used to understand exactly how the potential pharmaceuticals bound to the main protease. With that information, how the properties could be improved to make a pharmaceutical that was effective.

The detailed story was submitted in July of 2021 and published in Science by Owen et al., in the December issue of 2021. The X-ray data needed to understand and optimize the pharmaceutical targeting the main protease was collected at IMCA-CAT, the facility the Institute operates just outside of Chicago. IMCA stands for the Industrial Macromolecular Crystallography Association, an association of pharmaceutical companies committed to the use of macromolecular crystallography as a tool in drug discovery and product development. IMCA-CAT is the Collaborative Access Team defining both the beamline, entirely supported by the pharmaceutical industry, and the team that operates the beamline. The pandemic forced the shutdown of many activities in order to limit infection but working closely with management at the Advanced Photon Source, Dr. Lisa Keefe, the Executive Director of the IMCA-CAT worked out protocols that allowed the beamline to keep operating during the pandemic and enable the fight against COVID-19. This included protocols to handle sample shipments with minimal human contact, scheduling of operations such that a single staff member at a time was present, and automating aspects of the process so that much of the work could be done remotely. Hundreds of structures were produced, each using structural information from the previous one to improve the potential pharmaceutical properties. Extensive work was carried out before and after the structural studies, but our staff at IMCA-CAT played a small but critical role in in the fight against COVID-19 enabling Pfizer to use this structural information to produce Nirmatrelvir, one of the two pharmaceutical that make up Paxlovid.



A representation of the main protease in COVID-19 with structural components colored by helixes (red), sheets (yellow) and other chains (green). The inhibitor developed by Pfizer is colored blue.

It was important to the scientific effort against COVID-19 that synchrotron facilities were available and kept operating. While the number of potential commercial new pharmaceuticals being studied is kept private (but often in the hundreds per day), the beamline also works with the academic research community, and over 140 new biological structures were publicly produced by the beamline in 2020, and over 132 in 2021, a significant number for a facility of this kind, even without a pandemic impacting operations.

HWI was the leader in installing the *first-of-its-kind* Battery Energy Storage Systems (BESS) to meet the expected demand of our new Cryo-Electron Microscopy Center and provide power for the building during power outages. This was the largest indoor installation of BESS in the country and was possible because of the partnership with local companies Viridi and Stark Technology, and a tapestry of funding support.

POWERING

HWI's Groundbreaking Technology Revolutionizes Engery Storage

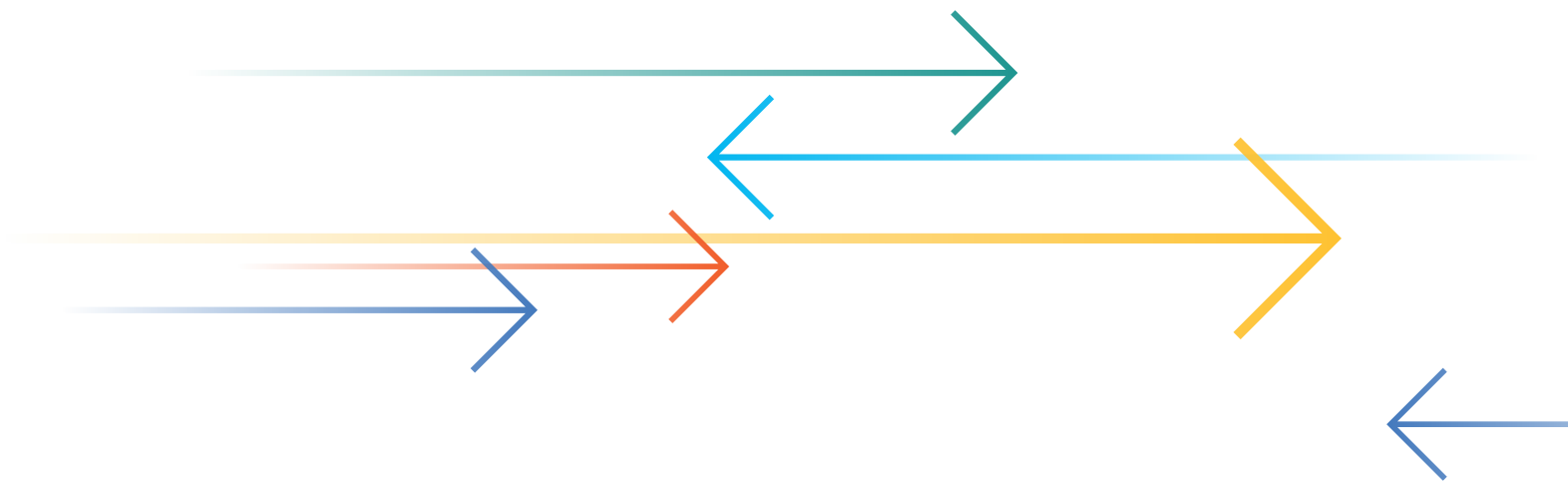
This project was a groundbreaking development in BESS technology. Viridi and HWI obtained approval under the then-fire code for the BESS installation. The system consists of twelve (12) 50kWh Lithium-Ion battery packs, which contain Viridi's patented anti-propagation technology – meaning Viridi removed the risk of fire in a thermal event, making it the safest BESS on the market. This was Viridi's first commercial installation of its BESS technology and, as stated in the NYS approval, "the storage system represents an opportunity for HWI and, in turn, the City of Buffalo to be on the cutting edge of energy storage in New York State." Jurisdictions across the country are analyzing this installation to craft future regulations and make this safe technology the standard. With a new development like this, HWI was able to commission a project with the University at Buffalo Department of Electrical Engineering. The engineering students determined that the battery system alleviated the need for a new transformer and power lines estimated to cost in excess of $500,000. The batteries charge at night and then release power during the day as demand warrants. This power can be released to HWI or back to the local grid. The study estimated a saving of $47,385 on electricity costs per year for HWI by using low-peak electricity and potentially selling electricity back to the grid.

HWI is extremely grateful to Viridi and Stark Technology, as well as help from the Buffalo Niagara Medical Campus, for working so closely on the development and installation of this project. We are grateful to Empire State Development, National Fuel Gas Distribution Corp., National Fuel Matching gift program, National Grid, Stark Energy Storage, and WNY Power Proceeds for their generous funding which enabled this battery development and installation locally. HWI has already had many visits from other potential customers to assess the technology.

THE FUTURE

The Battery Energy Storage System (BESS) shown above consists of 12 batteries plus sophisticated control electronics that provide the power storage for the system at HWI.

A perspective on the importance of worldwide



The theme for this Structures issue is journeys and it is rare for scientists to stay in the same geographical area throughout their career. I personally know of just a few exceptions to this. Moving laboratories used to be almost a requirement for career progression, and is seen a positive in providing a growth experience and exploring how different groups in different institutes pursue their science, both from an intellectual and a technical approach. As we explore different scientific environments, we encounter new technologies and new ways of thinking. We also connect with new members of a global network of experts.

In my case, I started my career with an undergraduate degree from Leeds (in England). Contrary to many, I stayed in Leeds for my PhD but I joined a highly interdisciplinary program based at the Astbury Center for Structural Molecular Biology. This was the beginning of my cross-disciplinary interaction. After graduating as a Structural Biologist focusing on cutting-edge crystallographic techniques, I moved to Hamburg (Germany) to expand my expertise into microfluidics. In Hamburg I encountered an even more global community, and I was able to explore synchrotron science (a high-energy physics machine use to generate X-rays) as we had an accelerator right on site (PETRA-III). After a few years in Hamburg, I was recruited to Buffalo, bringing the portfolio of experiences with me.

Looking back at my work, it is very clear that international collaborations were prominent in my science for over a decade. In one of my earliest publications, Dr. Edward Snell from HWI is in the author list. He jumped into the project to help elucidate the structure of my protein-protein complex in solution (rather than in a crystal), an expertise we did not have in our groups in Leeds. I have been collaborating with him since that first project over a decade ago. Moving to Hamburg, I kept my connections with the UK. The most striking work coming out of these contacts was the application of my new knowledge of microfluidics to the preparation of samples for Cryo-electron Microscopy (Cryo-EM). I had met Dr. Stephen Muench at the beginning of my PhD and we both had an interest in imaging protein dynamics. By sharing our respective expertise in

DIANA MONTEIRO, PhD

COLLABORATIONS

Gordon Research Conference, July 2022. Re-connecting with colleagues from Germany and the UK in person. In-person interactions were very limited through the pandemic.

BioXFEL conference 2019. BioXFEL is a National Science Foundation Science and Technology Center, bringing together scientists from around the globe.

Photo taken at the P14-2 experimental station (Hamburg, Germany). Pictured (from left to right) Dr. Michael Agthe, Dr. Diana Monteiro, Dr. David von Stetten and Ms Susanne Meier during a microfluidic sample delivery experiment in November 2019.

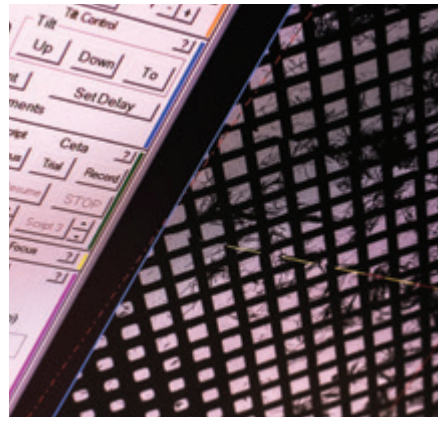
microfluidics and Cryo-EM, we lead a project that culminated in multiple publications and developed methods for alternative sample preparation pathways. Other collaborations grew over time, several of which arising from new connections at conferences.

Now at HWI, I still keep active collaborations with the UK and Germany, and my career has benefitted from many other worldwide contacts. Being part of a global community of scientists is imperative for both efficient scientific progress as well as establishing myself as a scientist through invited seminars and other contributions. These connections give me access to specialized infrastructure, such as the P14-2 endstation at PETRA-III, an one-of-a-kind experimental station dedicated to Serial and Time-resolved Crystallography. I still rely on European mentors for guidance, discussions, and support (and proof-reading!). Within this network of collaborators, we share infrastructure capabilities as needed, re-direct questions when we do not have a comprehensive answer to give ourselves and enrich the training of students and postdoctoral fellows.

I believe that science should be a global effort. COVID-19 showed what can be achieved when groups collaborate worldwide by sharing data and materials. The publications from pandemic science that had the highest impact show long lists of authors and groups, including scientists from HWI, all contributing to the same objective: learning how to fight a new, deadly disease. Worldwide collaborations increase scientific productivity as well as well-being. These contacts enrich our science as well as our own personal experiences by sharing customs and cultures.

Science is a journey, and it is a worldwide effort to make that world more healthy.

My journey is continuing and the experiences I gained at HWI have enabled me to move on from my position at HWI, joining the National Cancer Institute (National Institutes of Health) in Frederick, Maryland. I continue to collaborate with HWI groups, especially with Dr. Bowman and Dr. Lynch, making use of all of the capabilities offered by the National Crystallization Center.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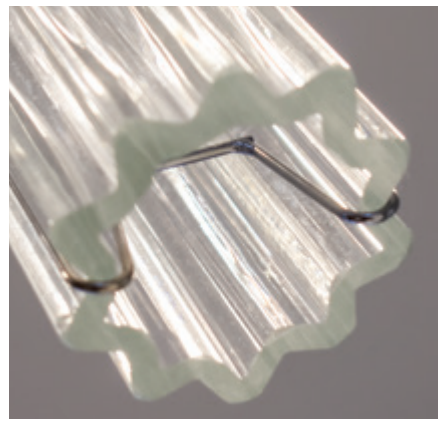

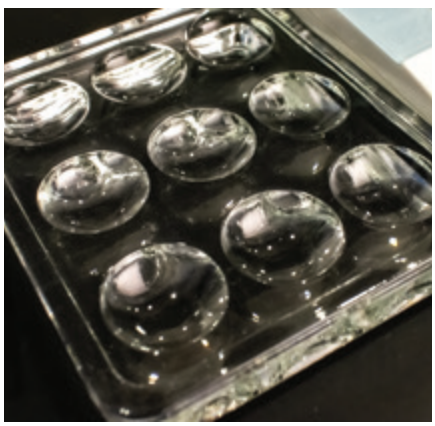

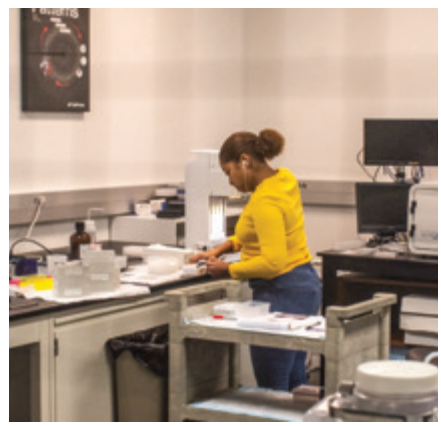

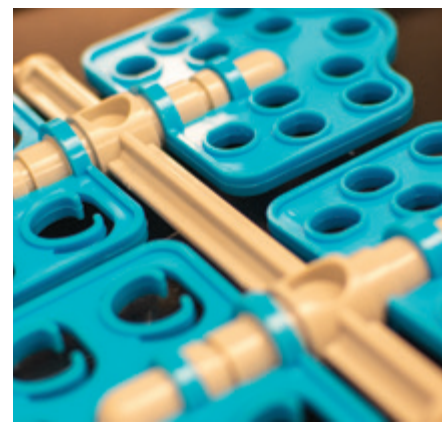

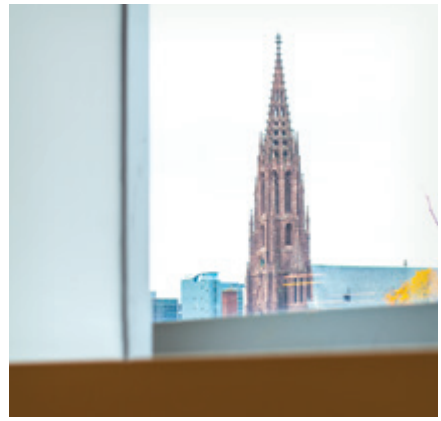

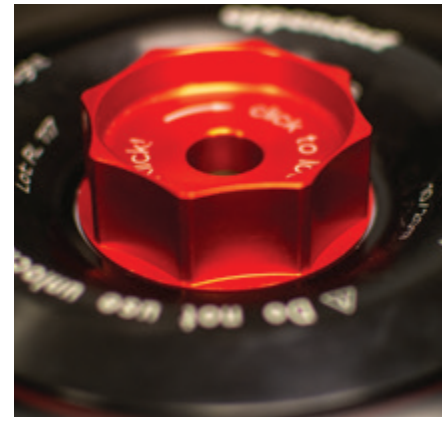
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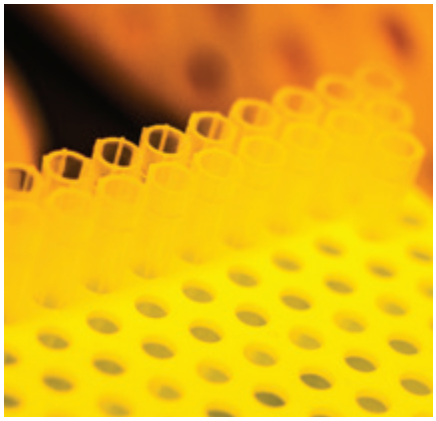


HWI


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PROTECT OUR ENVIRONMENT
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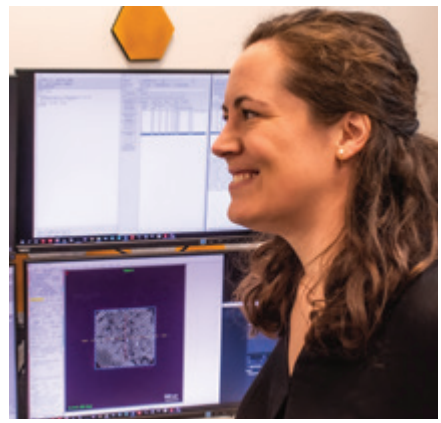
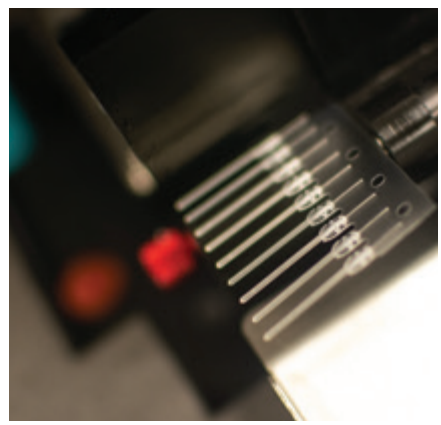
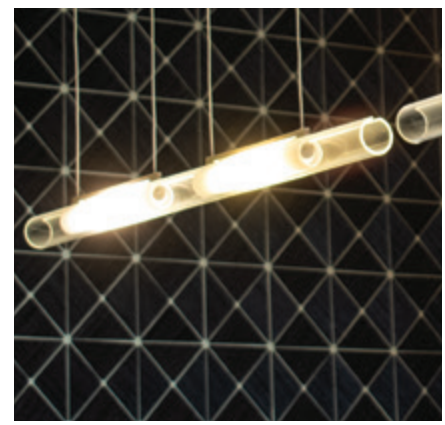






Welcoming new faces to the Institute

DR. GABBY BUDZISZEWSKI | Operations Manager at the National Crystallization Center

Dr. Budziszewski is a native Buffalonian who completed her bachelor's in biochemistry at Canisius College prior to moving to the University of North Carolina to complete her PhD in Biochemistry & Biophysics at the University of North Carolina at Chapel Hill working in the McGinty lab. She has expertise in macromolecular crystallography, recombinant protein expression and purification, enzymology, and biochemical assay development. She joined the HTX Center in Fall 2022. Dr. Budziszewski is passionate about working with users to develop strategies to produce diffraction-quality crystal hits and promoting an inclusive scientific work environment.

KELLY CAMPBELL | Director of Development

Kelly Campbell is a WNY native with over 10 years of experience working for a variety of non-profit organizations in the Buffalo/Niagara region. Prior to joining HWI, she served as the Development & Community Relations Director at Bertrand Chaffee Hospital and its foundation. During her time at BCH, Kelly managed internal and external communications, grew and stewarded relations with community partners, led government relations efforts, and raised funds through individual, corporate, foundation, and state supported giving.

Until 2019, Kelly served in the role of Planned and Major Gifts Officer at Meals on Wheels Foundation of WNY (FeedMore WNY) where she developed and implemented strategies to identify, cultivate, and steward individuals for significant gifts to advance the organization's mission and to assist donors in fulfilling their philanthropic goals. Additionally, she served as the Annual Fund Manager at the Buffalo Philharmonic Orchestra, where she coordinated the orchestra's $3.5 million annual giving program. Kelly is a graduate of SUNY Fredonia with degrees in both Music and Arts Administration.

DR. CHRIS CAMPOMIZZI | Research Associate

Dr. Campomizzi is a Rochester native and attended Niagara University receiving a B.S. in Biology. He then completed his PhD in Biochemistry at the University of Buffalo in the laboratory of D. Fernando Estrada, where he applied 19F-nuclear magnetic resonance to study cytochrome P450s, specifically CYP121 from Mycobacterium tuberculosis. During his time at the University of Buffalo, he received an American Society for Biochemistry and Molecular Biology Annual Meeting Award for an oral presentation in 2021, as well as the Biochemistry PhD Candidate Research Achievement Award for best dissertation in 2023. Chris is excited to join the Sarah Bowman group as a Postdoctoral Research Associate and expand his knowledge of structural biology techniques.

DR. SREESHMA NELLOOTIL SREEKUMAR | Research Associate

Dr. Sreekumar received a B.S. in Life Sciences-Zoology from Mahatma Gandhi University in India and a Master of Science in Biotechnology at Kannur University in India. She earned her PhD from Jamia Hamdard University by working at the International Centre for Genetic Engineering and Biotechnology in New Delhi, India. Prior to coming to HWI, she served as a Research Associate at Southern California Institute for Research and Education, Veterans Affairs, Long Beach Health Care System in California. During this tenure, her focus in Dr. Ling's lab was to identify novel therapies targeting Merkel cell carcinoma and tumor microenvironment.

Sreeshma has joined the Paz group and will be involved in projects focusing on structural-based understanding of the dynamics of key-human transporters, relating these to functional aspects of the transporters, and harnessing these insights into the development of novel therapeutic approaches. She is "really excited to work in the membrane protein world."

NICOLE TERRANOVA | Education and Diversity Director

Nicole Terranova has a career background in secondary education. She taught biology in California for 17 years, assisted in creating her school district's Next Generation Science Standards curriculum, developed social-emotional course content and student leadership curriculum content and activities while heading school events and student recognition programs. She completed her undergraduate work in zoology at University of California at Santa Barbara, obtained her teaching credential at California State University at Northridge, and acquired her masters in Curriculum and Instruction at California State University at Bakersfield.

She is working to create an effective community outreach program in Buffalo that helps more women and underrepresented minorities get into and excel in STEM career fields. Nicole has two children who are the never-ending source of fun and love that fuel her energetic spirit.

TIFFANY WRIGHT | Research Associate at the National Crystallization Center

Tiffany Wright joined the Crystallization Center at HWI in November 2022. New to the area of structural biology, she brings her experience to the lab from her background as a B.S. in Forensic Chemistry from Buffalo State College. Her work focuses on high-throughput protein crystallization, and she maintains daily operations and service output in the HTX Center.

MUCH LIKE HOW STRUCTURES INTERTWINE AND PROMOTE STABILITY, the relations and connections of individuals have ensured the stability and longevity of Hauptman-Woodward Medical Research Institute. The Hauptman-Woodward Medical Research Institute began as the Medical Foundation of Buffalo (MFB), thanks to the generous foresight and gift of $3 million from Helen Woodward Rivas in 1956. The genesis of the Medical Research Institute began as a chat between Helen and her friend Dr. George Koepf while doing dishes at a summer home in Honey Harbour, Ontario. She asked Koepf, an endocrinologist in Buffalo, if there was anything he dreamed of doing professionally that he was not already doing. He replied that he would like to study thyroid disease, which then resulted in the gift that funded the beginnings of MFB. That donation today would be worth over $30 million.

Leaving a legacy and ensuring the stability and longevity of Hauptman-Woodward Medical Research Institute was ingrained in Helen Woodward Rivas and continues to be in her family.

It was Helen Woodward Rivas' philanthropy and the combined vision of her and Dr. Koepf that set the foundation of what is today HWI as we know it—an institute committed to the science of structural biology and transformative research through education, discovery and innovation. Generations of Helen's family have continued her legacy of giving and supporting HWI through philanthropy, time, and talent.

Helen Woodward Rivas

Reid Stafford

Constance Stafford Constantine, granddaughter of Helen Woodward Rivas, notably served as Chair of the HWI Board of Directors, as well as the Chair of the capital campaign which funded the construction of HWI's current facility. During her leadership tenure, she established the Stafford Fellowship, funded by the Constance W. Stafford Trust (trustees: Walter F. Stafford III, PhD, Reid W. Stafford, Constance S. Constantine, and Robert Plache, Esq.), Drs. Walter and Sue Stafford, William and Margaret Constantine, and Walter and Constance Constantine. The fellowship has enabled six graduate students to grow their careers and contribute significantly to improving health. It has also enabled HWI to add state-of-the-art instrumentation to support its mission. The Fellowship, a permanent endowment benefiting HWI, and because of their generosity, their family will support educating scientists now and long into the future.

Constance W. Stafford, daughter of Helen, was instrumental in making sure that MFB was well funded after her mother suffered a debilitating stroke. She and her husband, Dr. Walter F. Stafford, were very generous, as well. She served on the Board of Directors for years and insisted that her daughter Connie join the Board. Dr. Walter F. Stafford III, a molecular biophysicist and grandson of Helen, has served on the Scientific Advisory Committee at HWI. Ted Constantine, Holly Constantine Ortman, and Emily Constantine Doren, great-grandchildren of Helen, have all been involved at HWI. Bill Constantine, brother-in-law of Constance Stafford Constantine, currently serves on the HWI Board of Directors, chairs the Development and Audit Committees, and serves on the Finance and Investment Committee.

The Institute has seen many changes over the years, the most dramatic being the recent hiring of new scientists, and seeing the rapid growth in their careers. We are extremely grateful to another descendant of our co-founder, Reid W. Stafford, who has followed this philanthropic spirit with philanthropy being an important part of his life. He donated over $2 million to the Institute to set up the Stafford Scientist program. This is to bring in new scientists to grow the impact of HWI and expand the breadth of diseases HWI is studying. This has a huge impact on the Institute and allows HWI to attract more scientists to join the journey in Buffalo. We are profoundly grateful to Reid W. Stafford for this recent donation, but also deeply saddened that he did not live to see the impact of his support. HWI is currently recruiting the first Stafford Scientist who will extend the legacy and impact of Helen Woodward Rivas, and help to make the world a healthier place.

Leaving a legacy and ensuring the stability and longevity of Hauptman-Woodward Medical Research Institute was ingrained in Helen Woodward Rivas and continues to be in her family. Fittingly, HWI established the Helen Woodward Rivas Society, a group for those have been inspired to make lasting gifts—planned gifts—to the Institute. Planned gifts allow you to make a significant gift while maintaining financial security for you and your family during your lifetime. Bequests, retirement plan designations, gifts of life insurance, gift annuities, and charitable trusts are just a few types of planned gifts. These gifts often provide attractive tax advantages and other financial benefits. They allow us to invest in new staff, and new ideas, and in addition to helping advance the capability of medical sciences, they bring funding and opportunities to Buffalo.

To learn more about how you can leave your legacy to Hauptman-Woodward Medical Research Institute and continue HWI's mission for generations to come, please contact:

Kelly Campbell, Director of Development
at 716-898-8624 or kcampbell@hwi.buffalo.edu.

BIOXFEL SUMMER INTERNSHIP

This summer, BioXFEL will once again have interns gaining invaluable scientific experience at HWI. In this 10-week summer program, interns will work with mentors at HWI and UB to become knowledgeable and experienced in protein crystallography so as to understand the initial necessary steps in creating samples that can be viewed by XFELs (X-ray Free Electron Lasers) in biological applications. This is the eleventh year that BioXFEL has had interns at HWI, while coordinating the summer internship with site coordinators and scientists at ASU, UWM, SLAC, and UC Merced.

The BioXFEL Summer Internship strives to increase the representation of underrepresented groups and women in XFEL sciences. This important avenue of scientific research has been crucial in viewing the structure of proteins thereby understanding their function, which has limitless applications in regards to drug interactions and cellular processes.

We are grateful that BioXFEL was awarded an extension to continue to further young scientist interest in STEM (Science Technology Engineering Math) careers and pursue future scientific research.

BioXFEL Summer Interns at SLAC

EDUCATIONAL DIRECTORS CONSORTIUM

"Teamwork makes the dream work."

JOHN MAXWELL

Surrounding HWI are numerous medical centers that each have their own educational directors incharge of engaging the community in what their center specializes in. The directors strive to disseminate the scientific research and medical practices that their center specializes in to increase adolescent awareness and potentially ignite a desire to pursue these scientific fields in their future careers. Creating educational opportunities in the form of outreach, programing, exhibit displays, etc., entails a symbiotic creation that honors scientific work while engaging a diverse audience.

Typically, medical centers have one or very few educational directors that must traverse a unique experience in creating their educational experience while intentionally increasing the diversity, equity and inclusion among the participants in their programs. As in most careers, it's beneficial to collaborate with coworkers that can provide insight and information that brings efficiency and ease to the position, as well as expand common thinking practices to be more "outside the box." Since this is not a frequent option for educational directions, finding collaborators requires looking outside their center to establish beneficial partnership(s). To address this need, the "Educational Directors Consortium" features an educational alliance between some of the educational directors from HWI, University of Buffalo, WNY STEM Hub, Roswell Park, Jacob's Institute, and the Collaborative Center for Social Innovation. The Educational Directors Consortium meet monthly to discuss opportunities to work collectively to promote comprehensive educational planning. A major focus that the directors discuss are successful methods to increase underserved groups and women interested in STEM fields while addressing equitable access to education and experiences that come with complex barriers. Another important matter that the consortium collaborates on is helping each other find suitable funding opportunities available to support our educational programs while examining opportunities to potentially pair up for grant applications to increase the likelihood to obtain financial support.

Ultimately, working collaboratively with others fosters creativity and support for all, and thesepartnerships strengthen educational programs by exchanging successful ideas as well as offering student visits to each center as part of these programs. These educational partnerships provide invaluable STEM education to Buffalo youth, thus strengthening the impact HWI and these centers make in WNY.

COLLABORATIVE CENTER FOR SOCIAL INNOVATION

ROSWELL PARK. COMPREHENSIVE CANCER CENTER

JACOBS INSTITUTE

HAUPTMAN–WOODWARD MEDICAL RESEARCH INSTITUTE

HEALTH EQUITY EDUCATIONAL EXPERIENCE SUMMER PROGRAM

WHAT WAS THE HEALTH EQUITY EDUCATIONAL EXPERIENCE SUMMER PROGRAM?

Last summer, HWI partnered with the Collaborative Center for Social Innovation (CCSI) in the creation of the new "Health Equity Educational Experience" this summer. This 8-week educational program provided an incredible opportunity for high school students to visit and have presentations from many of the centers around HWI, including BNMC, UB, Roswell Park, The Jacob's Institute, as well as the Buffalo Museum of Science to address the problem of "how can we improve cardiovascular disease rates in WNY?" This unique and comprehensive program allowed students to experience the multiple scientific perspectives and specialties that are needed to address such a complex health problem.

HOW DID THIS PROGRAM COME ABOUT?

This program was created by two prior science teachers that have recently left the classroom to continue their passion for engaging students in STEM careers in different ways. Our Educational and Diversity Director, Nicole Terranova, taught biology in California for 17 years, and although the classroom interaction with her students was rewarding and beneficial, she knew there were other scientific educational approaches that could provide students with a more realistic, impactful scientific experience. Nicole was fortunate to meet the founder of CCSI, Apryle Schneeburger, who was also a science teacher for many years who left the classroom to create her educational programming to bring about social innovation. Having similar career experiences and views of education allowed for an immediate cohesive vision of what a comprehensive, mindful educational program could be that includes HWI's research, as well as the medical expertise that the nearby centers provide. Passionate educators who seek to inspire future scientists can create outstanding opportunities for youth when the availability for them to visit so many amazing centers within a small proximity exists.

CONTINUES

HEALTH EQUITY EDUCATIONAL EXPERIENCE SUMMER PROGRAM CONTINUED

WHAT DID THE PARTICIPANTS LEARN IN THIS PROGRAM?

Throughout the Health Equity Educational Program, participants learned about a variety of content related to the cardiovascular system and the prevalence of its disease in WNY. Information regarding access to nutritional food sources based on location was examined as students learned the importance of mindful food consumption in its relation to heart health. The significance of exercise and lifestyle choices (in relation to substance use) was discussed in depth due to their great influence among teens. In regards to innovations created to remedy cardiovascular issues, students were informed about biotechnology advances produced by local centers. Learning about inherited genetic factors that may increase individual likelihood of detrimental cardiovascular conditions was vastly explored. Hormone involvement in regards to stress management was covered in detail so the students understood the importance of managing their stress in healthy ways to avoid adverse health effects. Vital soft skills were taught throughout the program including leadership, public speaking, problem-solving, iteration of solutions, teamwork, and communication.

WHAT WAS HWI'S ROLE IN THIS PROGRAM?

Woven into the educational content of the program was the vital role that HWI has in understanding protein structure in relation to nutrition, medication, hormones, enzymes, and more. Understanding basic structural biology helped the students see how blood pressure medications, blood thinners, etc. work by utilizing HWI's ability to view these medications at work to create cures. Examining health benefits to plant- based diets to synthesize necessary proteins was analyzed once students acquired basic understanding of proteins. HWI helped students understand how protein synthesis lends to examining nutrition at a molecular level so students could easily recognize the importance of HWI's research.

BESIDES SCIENTIFIC UNDERSTANDING, WHAT ELSE DID PARTICIPANTS GET FROM THIS PROGRAM?

Other important partnerships in this program addressed some of the diversity, equity and inclusion issues that can sometimes serve as barriers to access for opportunities like this. This program was available through the Erie County Summer Youth Employment Program to address some of these barriers so diverse groups of students could attend, by providing income by paying the participants minimum wage for their participation, as well as a free city bus pass for transportation and free lunch provided during each program day. In addition to the invaluable educational content and experience the participants attained through the program, they also received three sociology college course credits through Villa Maria upon completion.

WHAT WAS THE END GOAL OF THIS PROGRAM?

The culmination of this program entailed a public presentation by the participants at HWI in which they proposed their solution on how to improve cardiovascular disease rates in WNY using the information they learned and the experiences they had throughout the program. Students were expected to be implementers of constructive change after devising their culminating solution by enacting the knowledge they've obtained to inform their friends, family and community about how to develop and maintain proper heart health. All of the participating centers and locations had a representative from their site take part in the final presentations.

WHAT ROLE DID THIS PROGRAM HAVE IN THE FUTURE FOR BUFFALO YOUTH?

This program was integral in leading to similar comprehensive and extensive educational opportunities for Buffalo youth. With the ongoing demand for scientists nationwide, providing a variety of scientific viewpoints that weigh in on medical solutions and advancements is vital to triggering interest in STEM careers.

SEVEN QUESTIONS

NICOLE TERRANOVA

How does Buffalo tie into your past?

I was born and raised in Buffalo, and my family owned restaurants in WNY. After many years in the business, my family sold their restaurants in 2000, which freed them to move where they pleased. I was 20 years old at this time, and in my sophomore year at the University at Buffalo so I decided I was going to move with them. They decided that they wanted to move somewhere warmer that was also close in proximity to other relatives which brought us to Santa Clarita, CA.

How did you become interested in science?

I was fortunate to have a dad and grandfather that loved science. My father had a degree in botany and passionately discussed plants and nature often. My grandfather was very knowledgeable about wildlife, and I commonly accompanied him on outdoor adventures in which we would excitedly look for and talk about the animals we saw. Since I could pronounce the word "veterinarian," I wanted to be one, and my interest in helping animals persisted. I was also fortunate to have an enthusiastic third grade teacher who loved science whose passion helped to fuel my own.

What was your educational journey?

I started at the University at Buffalo for Computer Science and then switched to Biology. When I moved to California, I attended the University of California at Santa Barbara so I could get a degree in Zoology. After I graduated and started career job hunting, I decided to see if I would enjoy working with kids and during my substitute teaching interview, I was offered a full-time position in teaching life science, and two weeks later I was standing in front of a class of seventh graders wondering how it had happened! I obtained my teaching certification and a Masters in Sciences for Curriculum and Instruction, and then used my knowledge to assist my school district create the Next Generation Science Standards (NGSS) curriculum for all 7th grade students.

Where did your career lead you prior to HWI?

I taught for 17 years altogether in California which was an incredible career journey. I eventually became the Director of Student Activities at the school I worked at, which entailed running all school events, coordinating student recognition programs, creating a fundraiser to acquire school funds, and much more. I was also the school's yearbook advisor and video announcement class teacher. I also developed a passion for teaching students about the social-emotional skills that assist in career development.

What brought me back to Buffalo?

I greatly missed the "hometown" feel that I was lucky to grow up in and it saddened me that my children weren't experiencing a childhood similar to what I was fortunate enough to have here. I was also happy to come back to a large group of relatives and friends that I had dearly missed. 17 years of teaching was an incredible career that taught me more about myself than I could've ever predicted. However, I decided to step away from teaching and incorporate all I've learned into a related career that allowed for more creative control.

What hopes do I have for an HWI education program?

I'm looking forward to creating an effective community outreach program in Buffalo that helps more women and underserved groups get into and excel in STEM career fields. I'm excited to get students into HWI so they are familiar with the science we do here and are able to recognize its significance. I want to increase community relationships among the other institutions in BNMC so that all of our educational programs can thrive and better serve Buffalo youth. I also hope to increase HWI's community involvement by taking part in community events and creating educational pathways that provide opportunities for local students from underserved groups.

Favorite hobbies?

I have two children who are the never-ending source of fun and love that fuel my energetic spirit. Going on adventures with them and watching them grow into incredible people is a tremendous source of my happiness and where I most joyously allocate my time. I enjoy playing guitar and dabbling in art when I can. I enjoy almost anything DIY and fixing things, as well as cooking. I also enjoy spending time outside hiking and enjoying nature.

To learn more about HWI's Education Programs, please visit **hwi.buffalo.edu/education**.

CURES BEGIN HERE

FOR OVER 60 YEARS, Hauptman-Woodward Medical Research Institute has worked to find cures for diseases like COVID-19, cancer, and others that impact us today. Our renowned researchers study proteins in normal and diseased states and what they learn provides a foundation for developing medicines, therapies, and cures.

Hauptman-Woodward is Buffalo's only independent research institution and has an international reputation for excellence in structural biology. We house scientists in multiple disciplines and value diversity in ideas and backgrounds to promote novel and world-leading discoveries. Our goals of innovation, discovery, and education are driven by what we describe as CURE•OSITY as we work toward the cures of tomorrow.

INNOVATION // LEADING THE WAY

Our main funder has been the **NATIONAL INSTITUTES OF HEALTH** – We have also received competitive awards through **NATIONAL SCIENCE FOUNDATION, NASA,** and **THE DEPARTMENT OF DEFENSE.**

Since 2004, $89 million in federal grants have been invested in HWI research.

$89 MILLION

1.8

$2 MILLION

WAS RECEIVED FROM REID STAFFORD, WHICH IS ENABLING THE INSTITUTE TO BRING NEW SCIENTISTS TO HWI.

EDUCATIONAL IMPACT

$3 MILLION

THE INSTITUTE NOW PROVIDES **STRUCTURAL BIOLOGY SERVICES:**
WE ARE EXPERTS IN THE FIELD WITH OVER **60 YEARS** OF **EXPERIENCE**
WE ARE UNIQUELY POSITIONED TO DELIVER **SCIENTIFIC INSIGHT** TO **ENABLE RESEARCHERS** TO UNDERSTAND DISEASE BETTER.

$8.1 MILLION

WAS INFUSED INTO HWI'S CRYO-EM CENTER, WHICH INCLUDED A HIGHLY EFFICIENT PILOT GREEN SOLUTION FOR OUR BATTERY STORAGE COMPONENT.

HWI manages the IMCA-CAT group at **ARGONNE NATIONAL LABORATORY,** which is undergoing a massive upgrade to their facility beamline. While this is underway, we are conducting experiments at other facilities around the world. Once completed later next year, the IMCA-CAT group will have the vworld's premier industrial beamline.

IMCA-CAT
Industrial Macromolecular Crystallography Association Collaborative Access Team

THE INSTITUTE HAS $27 MILLION IN ASSETS.

HWI Scientists Identify Potential New Targets for Selective Drugs

DAN GERWITH, PhD

NEW DRUGS TO TREAT THE DISEASES OF THE MODERN WORLD ARE IN CONSTANT DEMAND. Sometimes these drugs are found by sifting through the bounty of nature, but increasingly the initial stages of drug discovery occur in the electronic highways and byways of the computer. This "in silico" screening can screen millions of virtual compounds against a "target" of interest. More often than not, the target is the 3D atomic resolution structure of a protein that is central to the disease or pathology being studied. For computer-based screening to work, however, the protein structure being targeted must be accurate in order to have a good picture of the three-dimensional landscape of the ligand binding site. Inaccuracy can take many forms, including, for example, a simple lack of high resolution. However, another class of variability comes from the protein target adopting new shapes in response to the binding of the drug.

The Gewirth lab at the Hauptman-Woodward Medical Research Institute studies such a shape-shifting protein, called Grp94. Using models the Gewirth lab generated from numerous X-ray crystal structures of its various conformations, they designed new inhibitor molecules to fit hidden pockets that are exposed when the protein changes it shape. Grp94 belongs to a class of proteins that are targeted not only for cancer therapies, but also potentially for diseases as diverse as Alzheimer's and microbial infections.

The most recent work from the Gewirth lab has focused on whether the selective drugs designed for Grp94 can be used to target members of the protein family found in different organisms. Leading this effort is Dr. Nanette Que, a senior staff scientist in the lab. Using precisely constructed protein chimeras, where parts of Grp94 are used to substitute for the equivalent region in another family member, Dr. Que has discovered the part of Grp94 that governs its shape shifting properties. Remarkably, this shape-shifting element is also found in the members of the family that come from bacteria or fungi. Since these proteins are essential for life in these organisms, this discovery opens the exciting prospect that the drugs initially developed to treat human cancers can be repurposed as potent anti-microbials to treat drug-resistant infections. While this is still a subject of further research, the work in the Gewirth lab has pioneered the prospect of exploiting the shape-shifting properties of Grp94 for the identification of new therapeutic strategies.

Gatekeepers in Our Body.

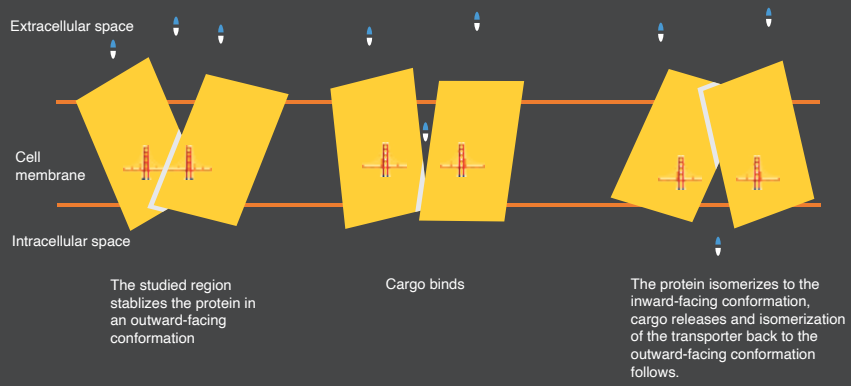
AVIV PAZ, PhD

Dr. Aviv Paz is working to help the development of new therapeutic approaches related to proteins embedded in the cellular membrane. Specifically, 60% of all drugs act on membrane proteins and many drugs that act on targets that reside in the cells are taken into the cells by membranal transport proteins. Dr. Paz's interest in these transport proteins and understanding how they work could be harnessed for the design and development of new drugs.

The body is made up of many living cells. Lipidic membranes form the boundary of these cells. These membranes form barriers between individual cells and between the cells and their environment. Some essential molecules passively penetrate these membranes, while other molecules cannot. If an impermeable molecule is necessary for the cell, or potentially acts as a drug to treat a disease, a specific membrane-embedded protein is tasked with binding this molecule from the outer environment of the cell, and shuttling it into the cell. To do so, this transport protein switches between different shapes, known as conformations. Broadly speaking, at the start of the transport cycle, the transporter is open towards the outside of the cell, exposing specific regions in the protein that attract the molecule and bind it. This is followed by a large-scale conformational switch that exposes the bound molecule to the inside of the cell, followed by the release of the cargo molecule inside the cell, and the return of the transporter to the outward-facing conformation in order to transport more molecules. An important factor in this transport cycle is that the transporter is never open simultaneously to the outside and inside of the cell, since this would cause a severe leak and uncontrolled flow between the cell and its environment, which could severely harm or kill the cell. While the broad picture of how this process occurs is known, detailed structural and functional knowledge necessary to fully understand the process and design new pharmaceuticals, is not.

Specific hinge regions that block the extracellular or intracellular paths that the cargo might take are called "gates". A recent study at the Paz lab identified one such gate based on structural models and characterized the gate in two related transporters from the Organic Anion Transporting Polypeptide (OATP) family, OATP1B1 and 1B3. These two transporters are expressed in the human liver and are essential for the uptake of various molecules and multiple commonly prescribed drugs, where these drugs are neutralized. The functional studies showed the identity and characteristics of specific regions of OATP1B1 and OATP1B3 that open and close during the transport cycle, controlling the seal formed by the transporter close to the intracellular region.

For the first time, this study demonstrated the involvement of these parts of the transporter in the shifting conformations of the OATPs by experimental and computational methods. Ultimately, these studies combined with additional functional and structural insights will enable us to form a better understanding of the discrete movements that occur during transport through different members of the OATP family and develop drugs that either activate or inhibit the OATPs. Activation of the OATPs is of importance since many chemotherapy agents act on targets that are inside the tumor cells and these drugs enter the tumors through OATPs, while the inhibition of the OATPs is important for preventing the cellular entry of some natural molecules that promote the progression of tumors.

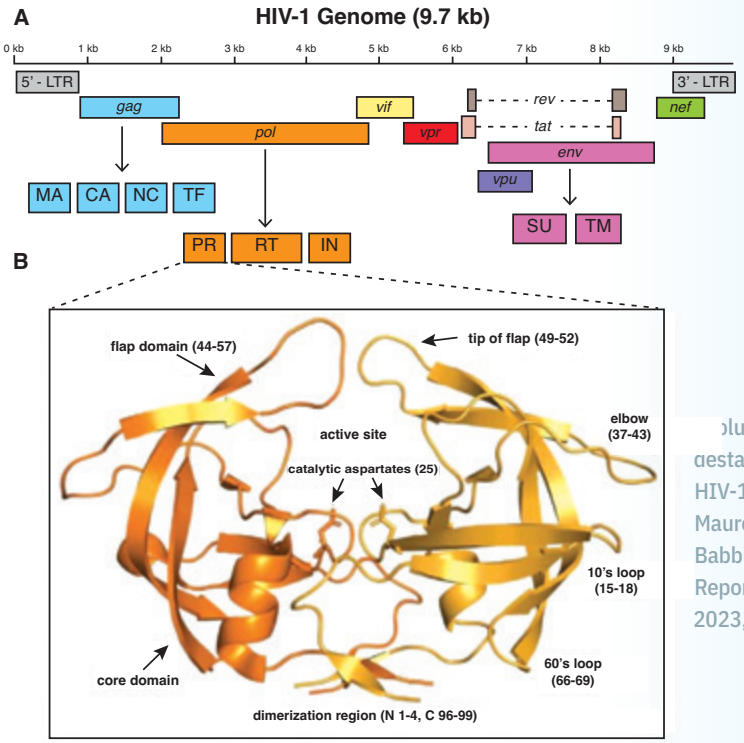


Dr. Paz's research, initially seeded by HWI Cureosity funds, is now being supported by a large federal grant from the National Institutes of Health and by the G. Harold & Leila Y. Mathers Charitable Foundation.

Fighting drug resistance in HIV/AIDS

MIRANDA LYNCH, PhD

Around the world, HIV/AIDS continues to be a major health problem. Several treatment regimens have dramatically reduced HIV-related illness and death. HIV-1 protease is one of the critical targets of these regimens. However, this drug target is prone to development of treatment resistance. In a study published in Biophysical Reports by HWI Assistant Investigator Dr. Miranda Lynch and collaborators at the Rochester Institute of Technology, machine learning-assisted comparative molecular dynamics methods were used to study changes in the target when a drug binds. The target had a 'flap region' where drug-resistant mutations accumulate. A key conserved region of that flap is impacted by drug-resistant mutations, impacting the ability for drugs to effectively interact with their target. This key finding suggests that drugs should be designed to target regions that are less dependent upon single sites with large functional binding effects. This will lead to future HIV therapeutics that are less prone to the rapid emergence of viral resistance.



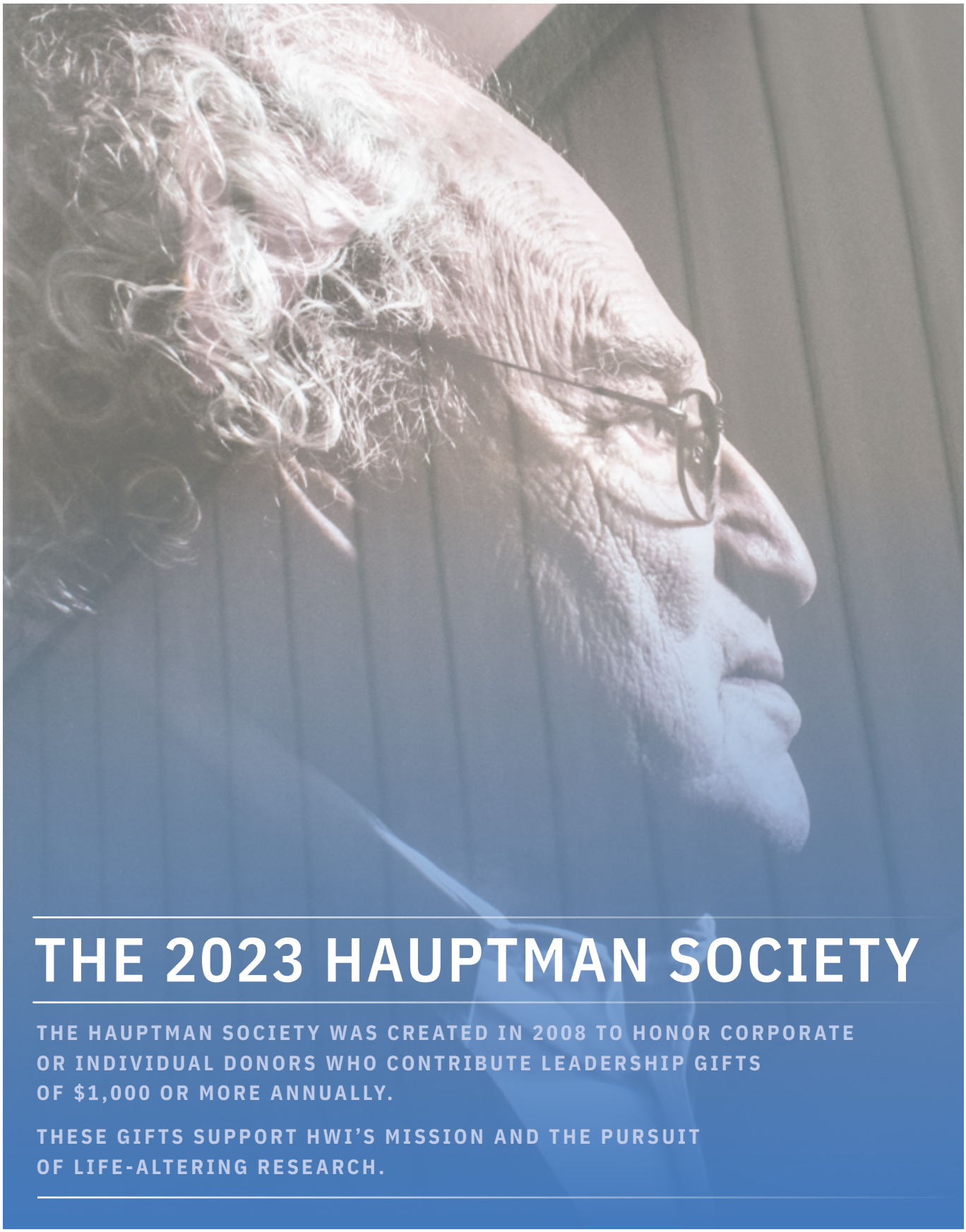
olution of drug resistance drives destabilization of flap region dynamics in HIV-1 protease, Madhusudan Rajendran, Maureen C. Ferran, Leora Mouli, Gregory A. Babbitt, and Miranda L. Lynch. Biophysical Reports. Volume 3, Issue 3, 13 September 2023, 100121

HWI YOUNG PROFESSIONALS is a six-session program that engages young professionals focused on building community support for Hauptman-Woodward Medical Research Institute.

Members have an opportunity to develop skills over the course of these sessions in areas such as networking, fundraising skills, board development, and community development. This group of young professionals will become ambassadors for Hauptman-Woodward in the community and help raise critical funds to advance our mission.

This year's class of Young Professionals is made up of individuals from a wide variety of professional sectors- banking, legal, staff recruitment, non-profit, and more. Their diverse backgrounds and skill sets have been a wonderful asset and have contributed in making this a robust experience.

If you are interested in joining our 2024 cohort or know of a great candidate please contact:
Kelly Campbell at kcampbell@hwi.buffalo.edu
or visit:
hwi.buffalo.edu/hwi-young-professionals-group.



THE 2023 HAUPTMAN SOCIETY

THE HAUPTMAN SOCIETY WAS CREATED IN 2008 TO HONOR CORPORATE OR INDIVIDUAL DONORS WHO CONTRIBUTE LEADERSHIP GIFTS OF $1,000 OR MORE ANNUALLY.

THESE GIFTS SUPPORT HWI'S MISSION AND THE PURSUIT OF LIFE-ALTERING RESEARCH.

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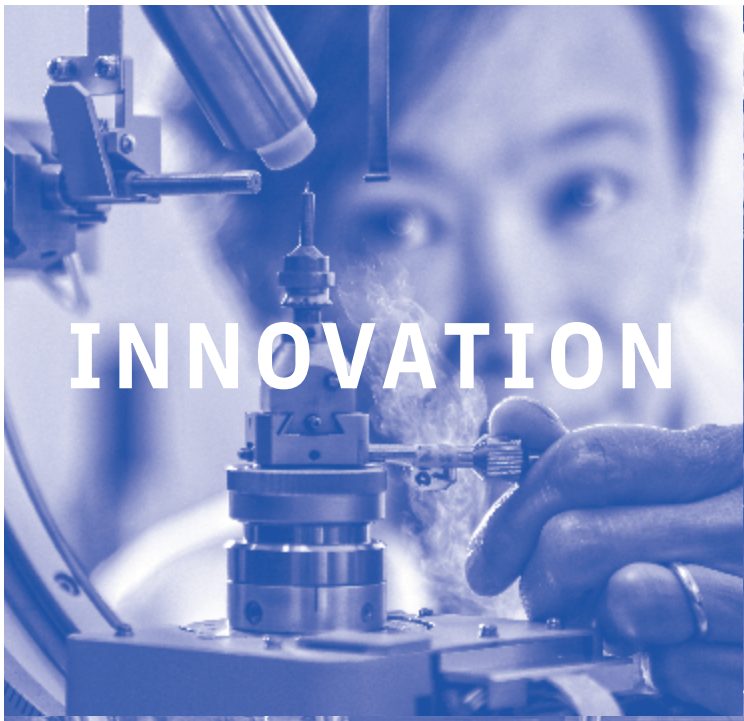
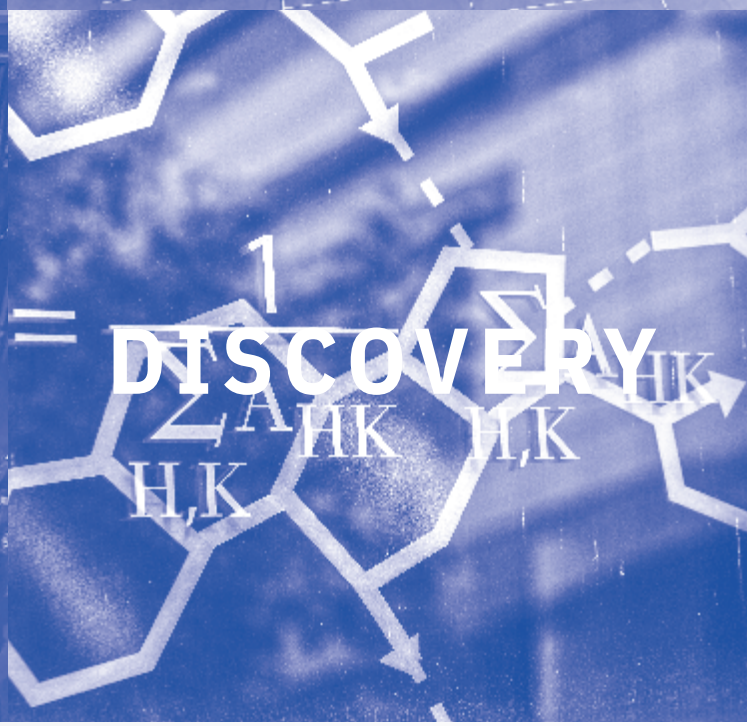




WAYS TO GIVE

HAUPTMAN-WOODWARD was founded because of philanthropy which then became a legacy for Helen Woodward Rivas. You too can make an impact in a multitude of ways and create your own legacy. We welcome you to contact HWI's Director of Development, Kelly Campbell at kcampbell@hwi.buffalo.edu or 716.898.8624 to discuss the numerous ways in which you can contribute and make a difference.

HAUPTMAN SOCIETY

The Hauptman Society was created in 2008 to honor corporate or individual donors who contribute leadership unrestricted gifts of $1,000 or more annually.

These gifts support HWI's mission and the pursuit of life-altering research. Membership advantages include our Annual member event, an invitation to exclusive speaker series, behind the scenes tour of HWI and the diffraction lab, upon request, and your name on the Hauptman Society plaque in the lobby.

MONTHLY GIVING

It is an easy, convenient, cost effective way to donate to HWI and make an impact. Your donation will be automatically charged to your credit card every month without you needing to do anything.

The same amount will be deducted on the same day of every month until you tell us you would like to increase, decrease or stop your donation.

PLANNED GIVING

A planned gift is a contribution that is arranged in the present and is allocated at a future date. These gifts historically for HWI have made significant impact at critical junctures in our history and we thank the donors who had the foresight of giving in this manner. Examples of planned gifts are listed below.

- Gifts of Appreciated Securities
- Gift of Personal Property
- Retirement Plan Gifts
- Life Insurance Gifts
- Gifts of Real Estate
- Planned Gifts
- Bequests
- Gift Annuities

IN MEMORY/HONOR OF

A donation to HWI is a thoughtful way to express your sympathy for the loss of a loved one or to honor someone special in your life or in the industry.

THE JANE F. GRIFFIN PhD EDUCATION FUND

This fund was established in 2016 to recognize HWI Emeritus Researcher Jane F. Griffin, PhD for her longstanding commitment to and establishment of HWI's education programs. The Griffin Fund supports undergraduate students with paid summer internships to work with HWI research teams and gain practical, hands-on experience in a research setting. Many students have gone on to publish results of their work from this program.

STAFFORD FELLOWSHIP

HWI has a rich history in educating the next generation of scientists. Fellowships permit new talent to be supported over the course of their studies with our world renowned research groups. The Stafford Fellowship, established by HWI Emeritus Board Chair Constance Stafford Constantine, is our longest standing fellowship and has supported numerous PhD candidates who are now prospering scholars. Donors can contribute additional funds to this fellowship that already exists.

ENDOWMENTS

Many individuals chose to contribute funds to the Institute that will ensure their gifts will continue to give for years, if not decades to come. For example, Funds contributed to an endowed chair recognize an individual or a family's legacy. Three endowed chairs exist at HWI that have varying missions, they are listed below. Contributions to these chairs which are not yet fully funded are a tremendous way to honor the spirit of both the mission of the chair and for who they are named.

Don and Vicky Hess Endowed Chair

The goal of the Donald and Victoria Hess Endowment fund is to raise permanent funds to further secure the financial strength of Hauptman-Woodward Medical Research Institute.

Herbert Hauptman Nobel Laureate Endowed Chair

This fund will support the work of an outstanding scientist whose work, echoing that of Dr. Hauptman, bridges the gap between pure science and biomedicine.

William L. Duax Endowed Chair in Crystallography

The purpose of the fund is to support the scientific work and teaching of Dr. William L. Duax, and of future generations of Hauptman-Woodward scientists.

Create your own endowment

Endowed Funds can be used to establish a chair that will enable HWI to recruit the very best scientist who will have discretionary income to support their efforts from the chair they hold.

You can read more about these opportunities on our website at hwi.buffalo.edu/giving

EDWARD SNELL, PhD

Diversity Drives Discovery

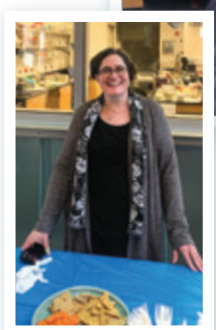
The vision of HWI is to improve the health and well-being of humanity through structural biology with innovation, discovery, and education. Humanity is diverse, and we, as an organization, need to be equally diverse to achieve success in our vision. While science is broad, progress is only made on those questions that we think to ask. The background of a scientific team shapes those questions. For example, studies show that Black scientists are more likely to study health disparities than white scientists, and female scientists are more likely to study pregnancy and education than are male scientists. While the scientific method strives to be impartial, our background shapes our thinking.

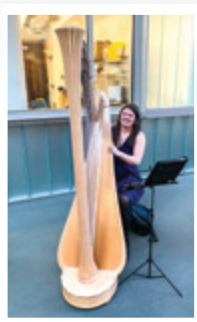
Over the nine years I served as CEO at HWI, we've made great strides in changing the demographic of our scientific teams and staff by focusing on ways to open science to a wide community and being aware of barriers that may not be obvious. Structural biology has always been seen as an egalitarian home for many, with women making distinguished contributions. Of the eight women who have won the Chemistry Nobel, four make use of structural biology: Dorothy Hodgkin, Ada Yonath, Frances Arnold, and Jennifer Doudna. There will be many more. The name Rosalind Franklin is well-known for providing the experimental data that revolutionized our knowledge of biology and the discovery of the helix structure of DNA. She also carried out important work on carbon and on plant and animal viruses.

For over six years, I have served on the International Union of Crystallography Gender Equity and Diversity Committee. I'm honored that they asked me to serve another three-year term. This opportunity has provided an interesting background and informed discussion group to discuss best practices, especially where the organization is small. Quietly, we've been increasing awareness of diversity and inclusion. The most significant effort started when we began working with Puerto Rico students over 10 years ago and realized there was a pool of talented students but with limited resources. We were able to help break down barriers to entry, we hosted students here in Buffalo, and even brought their families to Buffalo when hurricanes and earthquakes struck the island. We have become friends with many and we follow their blossoming careers at places like Stanford and Yale. We are now looking at ways to implement a similar effort with local populations and provide pathways into biotechnology careers for local underserved groups.

Our Education and Diversity Director, Nicole Terranova, introduced a display board in our lobby that celebrates diversity. She engages in local DEI initiatives such as Juneteenth and community cleanups and works closely with the Buffalo Niagara Medical Campus and their goal to create "a vibrant, culturally relevant hub where diverse communities connect and thrive". If you view our staff and Board of Directors pages on our website, you'll notice demographic diversity among these individuals. Our young professionals' group has conducted meetings on the subject of DEI. Diversity is across the organization with many of our staff members involved in discussion groups and events, e.g. attending the Annual Biomedical Research Conference for Minoritized Students. We plan to continue and grow these efforts. Our background shapes our thinking, so we want that background to be as broad as possible. Our research at HWI impacts everyone, and we want everyone to be represented in that research.

OUR ANNUAL COOKING SERIES





In March 2023, HWI hosted the first in-person Cuisine de Laboratoire, except this time the highlight was our HWI staff and scientists served as our chefs for the evening! Attendees not only had the chance to taste excellent food, but they also were able to meet and interact with our HWI team in a unique way.

In addition, thanks to the generous sponsorship of Mr. and Mrs. William Constantine and Bank of America, Nile Restaurant from the West Side Bazaar was also on hand, serving their famous samosas and other delicious food to our guests.

HWI is committed to helping the WNY community. This year's Cuisine event was a special opportunity for us to give back by aiding a business impacted by the September 2022 fire at the West Side Bazaar.

Thank you to all those who attended and helped support this special event.

HWI TAPS INTO BUFFALO´S BEST

The Hauptman-Woodward Medical Research Institute is proud to have a diverse and active board that helps to guide and ensure that our activities make the biggest impact on the health of the world. In this issue, we introduce our new board members.

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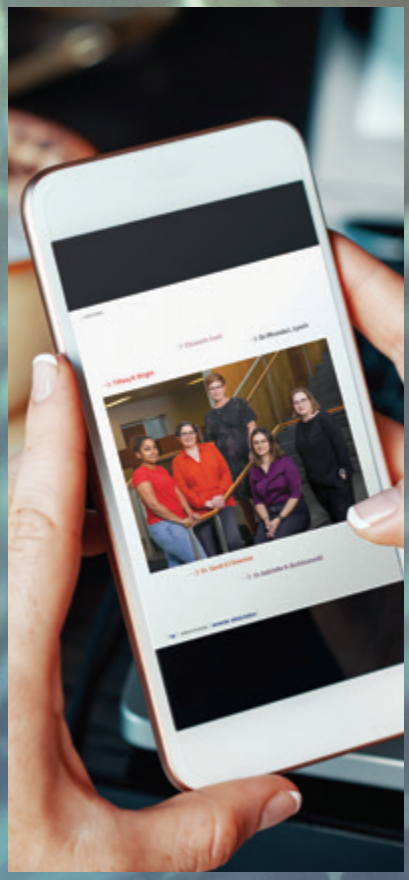

READ STRUCTURES WHEREVER YOU ARE.

Explore the digital magazine at
hwi.buffalo.edu/structures-magazine

HAUPTMAN–WOODWARD
MEDICAL RESEARCH INSTITUTE