

TECHNOLOGY INNOVATION PROGRAM 2023



BIG SCIENCE. BIG IMPACT.

Oak Ridge National Laboratory is the Department of Energy's largest multidisciplinary laboratory, delivering scientific discoveries, technical breakthroughs, and scientific user facilities to address pressing challenges in energy, the environment, and national security.

The Laboratory is home to more than 6,000 scientists, engineers, technicians, and support staff representing more than 70 nations. We are driven by our shared purpose to meet the world's biggest challenges with intelligence, creativity, and teamwork.

ORNL researchers apply unique facilities, sophisticated tools, and signature strengths in neutron science, high-performance computing, advanced materials, biology and environmental science, nuclear science and engineering, isotopes, and national security research to benefit science and society.

Established in 1943 as part of the Manhattan Project, ORNL continues to build on a legacy of scientific discovery in service to our nation.

MISSION

Deliver scientific discoveries and technical breakthroughs needed to realize solutions in clean energy and national security and provide economic benefit to the nation

VISION

Oak Ridge National Laboratory is the world's premier research institution, empowering leaders and teams to pursue breakthroughs in an environment marked by operational excellence and engagement with the communities where we live and work.

TECHNOLOGY INNOVATION PROGRAM

Oak Ridge National Laboratory is helping to speed new technologies to market while also building supportive and resilient ecosystems to the benefit of our local, state, and national communities.

The depth and breadth of our wide-ranging, world-leading expertise and facilities are unparalleled and provide a competitive advantage to our partners. The Technology Transfer team is driven by a shared mission to connect the lab's unique strengths in scientific discovery, clean energy technology, and national security to the world's biggest challenges.

ORNL's Technology Innovation Program accelerates commercial adoption of promising lab-developed technologies by making targeted investments that enhance commercial readiness and raise a technology's visibility. Since 2012, ORNL has invested more than \$11 million in 49 projects, resulting in 37 commercial licenses and options with partners ranging from Fortune 100 companies to early stage startups.

The 2023 cohort of TIP technologies includes:

- Ultraclean condensing furnace, Zhiming Gao, Buildings and Transportation Science Division
- Rapid droplet sampling interface, Vilmos Kertesz, Biosciences Division
- Closed-cell insulation foams enabled by coated and evacuated nanoporous materials, Meghan Lamm, Manufacturing Science Division
- Mixed plastic recycling by a tailored organocatalyst, Tomonori Saito, Chemical Sciences Division
- Accelerating the development of orally bioavailable therapeutics for beta-coronaviruses with structure-based molecular design, Brian Sanders, Biosciences Division

Additional presentations include:

- Unintrusive building leakage visualization and measurement using background oriented schlieren photography, Philip Boudreaux, Buildings and Transportation Science Division
- Methods for immunoregulation by modulating plasminogen-apple-nematode (PAN) domain-containing proteins, Wellington Muchero, Biosciences Division



Zhiming Gao

Buildings and Transportation Science Division

Zhiming Gao is a senior research and development staff member in the Buildings and Transportation Science Division. His research primarily focuses on developing energy-efficient HVAC equipment, including furnaces, heat pumps, water heaters, desiccants, and membrane applications. Gao's R&D work in exploring novel catalyst materials and designing compact acidic gas reduction catalyst components led to the development of a clean and efficient furnace, which received an R&D 100 Award in 2022.

Publications

Gao, Zhiming, et al. "Nondestructive neutron imaging diagnosis of acidic gas reduction catalyst after 400-Hour operation in natural gas furnace." *Chemical Engineering Journal* 454 (2023): 140099.

Gao, Zhiming, et al. "Ultra-clean condensing gas furnace enabled with acidic gas reduction." *Energy* 243 (2022): 123068.

Intellectual Property

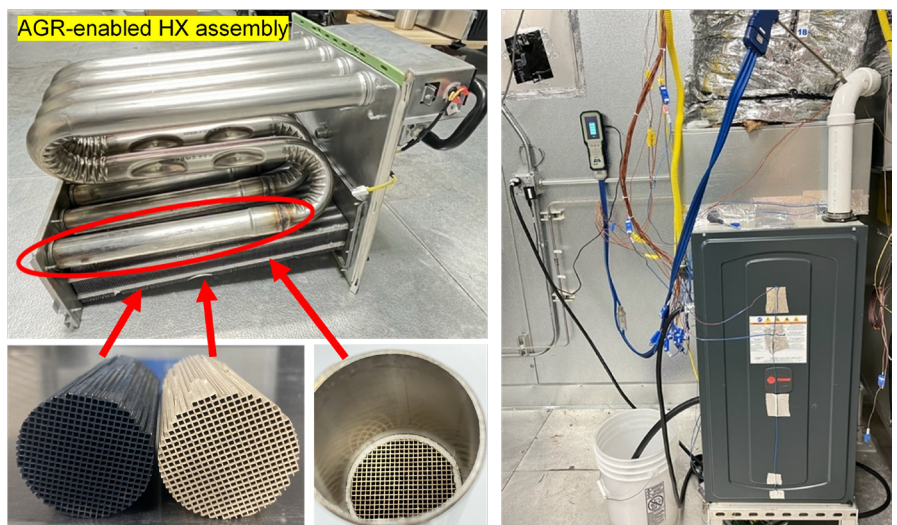
"Advanced Adsorption Technology for New High-Efficiency Natural-Gas Furnace at Low Cost," Invention Ref. No. 201804153
US Patent Application 17/232,274, filed April 16, 2021

Ultraclean Condensing Furnace

Problem: Residential natural gas furnaces are widely used for space heating in US homes. However, the acidic components in furnace combustion gases, such as sulfur oxide, nitrogen oxide, and formic gases, pose a significant environmental challenge. In particular, the acidic gases combine with water vapor to form an acidic condensate with a pH of about 3, which is more acidic than typical acid rain. The acidic condensate leads to corrosion and fouling problems. Furnace manufacturers and utility customers are actively seeking a solution that eliminates acidity in furnace condensate, reduces emissions, and achieves high efficiency and simplified installation.

Solution: The Ultraclean Condensing Furnace addresses these challenges. By incorporating compact and cost-effective acidic gas reduction (AGR) components, the technology achieves ultraclean flue gas and neutral condensate. The novel furnace design can remove more than 99.9% of acidic gases and other emissions, including trapping over 95% of sulfur oxide, reducing over 95% of nitrogen oxide, and oxidizing formic acid, carbon monoxide, hydrocarbons, and methane by nearly 100%. This results in the discharge of neutral condensate. The neutral condensate allows for a simpler and less expensive furnace design by utilizing a large low-cost secondary heat exchanger. That enables ultrahigh furnace efficiencies and eliminates the need for an acidic condensate treatment system.

Impact: The Ultraclean Condensing Furnace has the potential to revolutionize the residential heating market. With the majority of 118 million homes in the US relying on natural gas furnaces, the technology's impact on environmental emissions can be substantial. The AGR-enabled furnace achieves ultralow emissions compared to the US EPA furnace standard. Additionally, the absence of carbon monoxide emissions substantially simplifies American National Standards Institute certification for original equipment manufacturers and allows for safer operating conditions. The neutral condensate enables a simpler and more cost-effective furnace design, providing higher efficiencies and eliminating corrosion concerns. The applicability of AGR and clean furnace technologies can extend beyond residential condensing furnaces to other natural gas HVAC devices.



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Vilmos Kertesz

Biosciences Division

Vilmos Kertesz is a senior research and development staff member in the Biosciences Division. His research focuses on the development and application of novel high-throughput and surface sampling mass spectrometry techniques to chemically characterize liquid samples, single cells, and animal and plant tissues at small spatial scales. Kertesz's work on developing novel high-throughput sampling techniques led to the development of the RDSI technology.

Intellectual Property

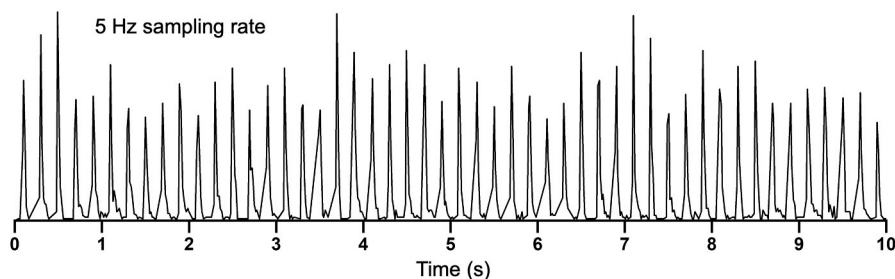
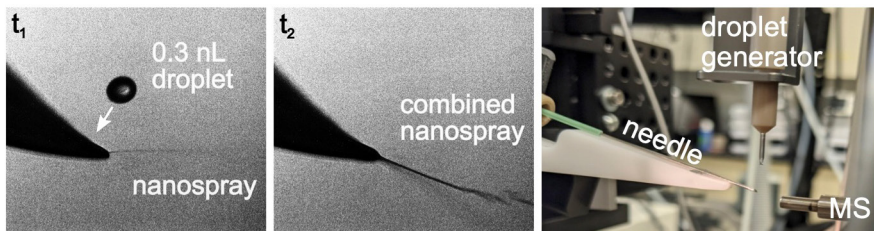
"Rapid Droplet Introduction Interface (RDII) for Mass Spectrometry," Invention Ref. No. 202004712
US Patent 11,651,945, issued May 16, 2023

Rapid Droplet Sampling Interface (RDSI)

Problem: Chemical characterization of liquid samples is a common need across a variety of research industries, including the pharmaceutical, biochemical, clinical, and environmental sectors. However, with current technologies, liquid samples often require vigorous sample processing procedures, which extends the total analysis time and costs. Methods to improve cost efficiency and sensitivity while retaining high sampling throughput are highly desired in the biochemical, pharmaceutical, and medical research communities.

Solution: The Rapid Droplet Sampling Interface (RDSI) is a versatile, ultrahigh-throughput, and ultralow-volume chemical analysis method. This novel methodology enables chemical analysis of samples at speeds up to five samples per second through droplet ejection and capture in a continuously flowing open solvent stream coupled with mass spectrometry analysis. By using droplets of the sample, measuring chemical composition requires as little as a few nanoliters. The continuously flowing solvent stream ensures the minimal sample-to-sample carryover and stable ion generation necessary to achieve quantitative analysis at high frequency.

Impact: The RDSI technology addresses the sensitivity, speed, and material cost shortcomings of competitive rapid analysis technologies by providing ultrahigh-throughput chemical analysis while drastically reducing associated costs. The RDSI will allow quicker turnaround in both pharmaceutical and clinical laboratories that in turn can yield faster drug discovery and disease diagnosis. The RDSI can be coupled with any droplet dispensing system, enabling varied sampling capabilities and application areas. These collective features of the RDSI make it primed to affect society by transforming high-throughput sampling and analysis in multiple areas of the analytical branch of the health sector.



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Meghan Lamm

Manufacturing Sciences Division

Meghan Lamm is an associate research and development staff member in the Manufacturing Sciences Division. Her background is in polymer chemistry with a focus on structure-property relationships. Her research focuses on the development and application of sustainable manufacturing technologies with a focus on biobased materials as alternative feedstocks and the building and transportation sectors. Dr. Lamm's work on insulation materials, focused on structure-property relationship in the materials, led to the development of the closed-cell nanoporous thermoset foam insulation technology.

Publications

Lamm, M. E.; Li, K.; Atchley, J.; Shrestha S. S.; Mahurin, S. M.; Hun, D.; Aytug, T. Tailorable thermoplastic insulation foam composites enabled by porous-shell hollow glass spheres and expandable thermoplastic microspheres. *Polymer*. 2023, 267, 125652.

Intellectual Property

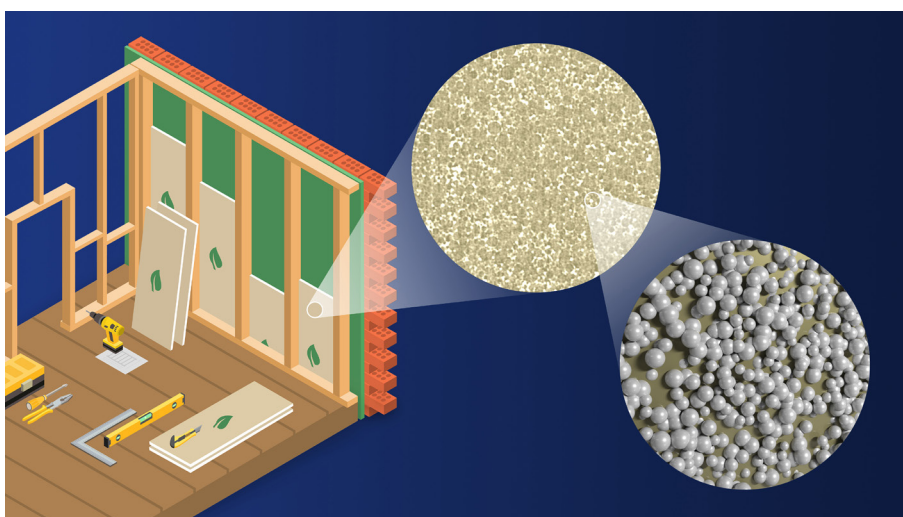
"Coated Hollow and Evacuated Insulation Particles (CHEIPs)," Invention Ref. No. 201804138
US Patent Application 17/384,317, filed July 23, 2021
US Patent Application 17/509,869, filed October 25, 2021
"Industrially Processable Thermoset Foam Insulation Dough," Invention Ref. No. 202305345

Closed-Cell Insulation Foams Enabled by Coated and Evacuated Nanoporous Materials

Problem: Maintaining temperatures within the building and transportation sectors accounts for more than 40% of global primary energy consumption. Therefore, there is a strong need for sustainable and high-performance thermal insulation technologies that can reduce energy loss, increase indoor space and building longevity, and improve carbon performance of buildings compared to conventional insulation materials such as thermoplastic and thermoset foams as well as vacuum insulation panels (VIPs).

Solution: The buildings sector needs energy-efficient, slim, low-cost, and robust building envelope solutions to help maintain thermal comfort. Based on industrially relevant processes, ORNL closed-cell thermoset foam insulation technology combines dual hollow filler materials embedded in a thermoset matrix. Currently, this technology platform enables good insulation performance ($R/in. \geq 5$), customizable insulation density, and robust mechanical properties and is expected to have better fire and smoke retardancy, all of which are attainable with an easily scalable, more environmentally friendly, and cost-effective fabrication process than commercial thermoset or thermoplastics foam insulation materials.

Impact: As the worldwide demand for energy savings calls for improvements in thermal performance, stricter standards such as the passive house and zero-energy concepts are necessitating development of new insulation materials. With an attractive value proposition of industrially scalable and manufacturable formulations and processes, integration of the ORNL technology into the insulation markets, replacing both the conventional and VIP systems, would provide significant economic and environmental benefit. A range of industries could easily adopt this cost-effective, high-performance, and customizable solution. The technology will decrease end-use energy consumption and allow for increased indoor space by reducing the thickness of building components, a valuable aspect for consumers.



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Tomonori Saito

Chemical Sciences Division

Tomonori Saito is a senior scientist in the Chemical Sciences Division. He leads multiple polymer science projects at ORNL, and his team has developed multiple technologies related to plastic recycling. Because of his inventions, he was named ORNL Inventor of the Year by Battelle in 2023. He has published more than 120 peer-reviewed articles, holds 13 patents, has had several technologies licensed to industry, and has won R&D 100 Awards in 2012, 2016, 2019, and 2021.

Publications

Md. Arifuzzaman, Bobby G. Sumpter, Zoriana Demchuk, Changwoo Do, Mark A. Arnould, Md Anisur Rahman, Peng-Fei Cao, Ilja Popovs, Robert Davis, Sheng Dai, Tomonori Saito "Selective deconstruction of mixed plastics by a tailored organocatalyst" under review Materials Horizons.

Intellectual Property

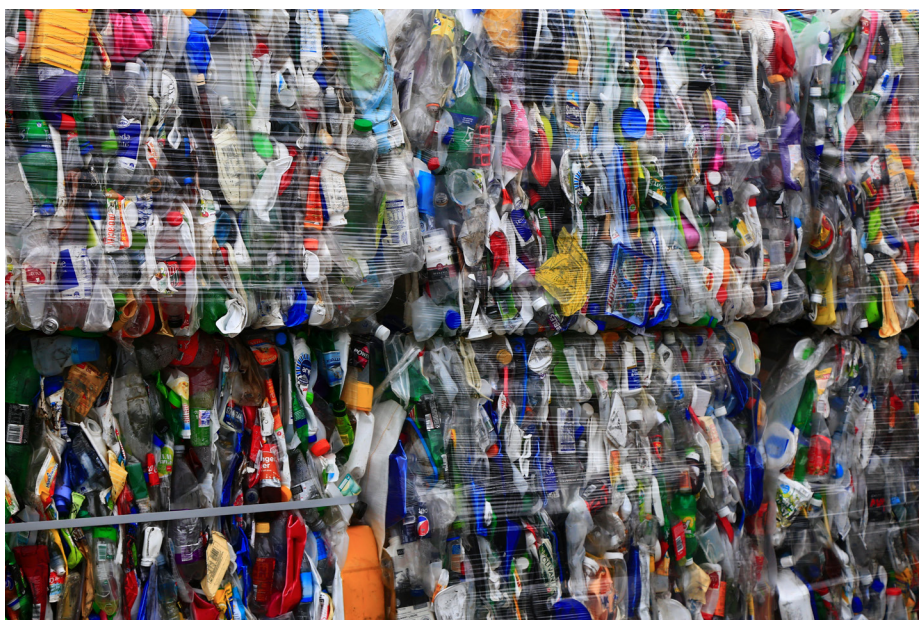
"Methods of Mixed Plastic Recycling enabled by a Highly Efficient Organocatalyst," Invention Ref. No. 202205137
US Patent Application 18/096,849, filed January 13, 2023

Mixed Plastic Recycling by a Tailored Organocatalyst

Problem: Plastics have numerous benefits in our lives, but plastic waste management has become a global environmental crisis. Approximately 80% of the more than 400 metric tons of plastics produced annually is improperly disposed, which equates to \$100 billion worth of materials being lost. Only 9% of plastic waste is recycled, most of which is downcycled into lower value products. Plastic waste-to-product solutions that are efficient and cost-effective are needed to convert plastic trash to clean value-added commodities.

Solution: ORNL's mixed plastic recycling technology can simultaneously break down various condensation polymers such as polyesters, polycarbonates, polyurethanes, and polyamides into monomers in a low-energy green process. The developed novel catalyst can deconstruct condensation polymers at 100% conversion within two hours and be reused multiple times, which is far superior to state-of-the-art organocatalysts. This technology can be used to deconstruct various types of plastic waste such as bottles, packaging, foams, mattresses, protective gear, automotive components, textiles, and more into chemicals, which can be made into virgin polymers. Other plastics that are not deconstructed in this process can be filtered, collected, and reused.

Impact: The developed technology enables single-batch, mixed waste plastic deconstruction and production of valuable chemicals from various unrecyclable plastics with exceptional efficiency. This technology offers new opportunities to solve the problems surrounding waste management and chemical manufacturing. Since the inability to deconstruct mixed plastics has prevented wide industrial adoption in converting waste plastics to chemicals, this technology could lead to a transformation of plastic recycling. This process will not only reduce plastic waste entering landfills but will also add significant commercial value to current plastic wastes, opening a new paradigm of plastic recycling toward a net-zero carbon society.



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Brian C. Sanders

Biosciences Division

Brian Sanders is an associate staff scientist in the Biosciences Division. His research focuses on chemical biology and bioconjugation for the development of anti-viral and anti-cancer therapeutics and for understanding plant-microbe interactions. In close collaboration with Jerry Parks—also of the ORNL Biosciences Division—Sanders has used clever molecular design, computational screening, and synthesis to develop promising therapeutic leads for antiviral drugs.

Publications

Sanders, B. C.; Pokhrel, S.; Labbe, A. D.; Mathews, I. I.; Cooper, C. J.; Davidson, R. B.; Phillips, G.; Weiss, K. L.; Zhang, Q.; O'Neill, H. ... Parks, J.M. Potent and selective covalent inhibition of the papain-like protease from SARS-CoV-2. *Nat. Commun.* 2023, 14 (1), 1733.

Intellectual Property

"Development of Covalent Inhibitors of the Papain-like Protease from SARS-CoV-2," Invention Ref. No. 202004743 US Patent Application 17/896,182, filed August 26, 2022
PCT Application PCT/US2022/041629, August 26, 2022

Accelerating the Development of Orally Bioavailable Therapeutics for Beta-Coronaviruses with Structure-based Molecular Design

Problem: There is a critical need for new antiviral drugs for treating infections of severe acute respiratory syndrome-coronavirus-2 (SARS-CoV-2). New drugs are crucial for rapid therapeutic response to COVID-19, supporting ongoing vaccination campaigns, and expanding future antiviral drug options. SARS-CoV-2 variants can evade vaccines and antibody treatments; new variants continue to emerge and are expected to cause future outbreaks. The problem is relevant to national and global public health and is specifically important to economic stability and national security.

Solution: Through rational and computational design, an ORNL team developed a potent and selective covalent inhibitor of the papain-like protease (PLpro) of SARS-CoV-2. PLpro is a critical target because it is essential for viral proliferation and dysregulates the host immune response. The team's best lead to date has a half-maximal inhibitory concentration of 38 nM and half-maximal effective concentration in multiple SARS-CoV-2 variants ranging from 0.32–1.3 μM in vitro. New compound designs will further improve metabolic stability and oral bioavailability.

Impact: A successful therapeutic could capture a significant percentage of the total coronavirus current and future therapy market. Investments from domestic and international governments for preparedness stocks for future novel coronavirus outbreaks offer potential revenue. There has been a significant loss of life due to SARS-CoV-2 infections over the last three years, upwards of 6.8 million lives lost. Accordingly, there is a desperate need for new antiviral drugs that would have an enormous societal benefit on global health, security, and economics.



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Philip Boudreaux

Buildings and Transportation Science Division

Philip Boudreaux is a research and development staff member in the Building Envelope Materials Research Group. His training and early career experience is in physics and optics, including work on a non-invasive skin cancer detection system and hyperspectral refractometer for clear liquids. Since 2008 he has been working in the building research area. Over the past few years, he has been able to apply his past optics expertise to buildings. He is working on non-intrusive testing techniques so that building performance assessment can be done easier, quicker, and cheaper.

Publications

Boudreaux, P., Venkatakrishnan, S., Iffa, E., and Hun, D. 2022. "Application of reference-free natural background oriented schlieren photography for visualizing leakage sites in building walls." *Building and Environment* 223, 109529.

Intellectual Property

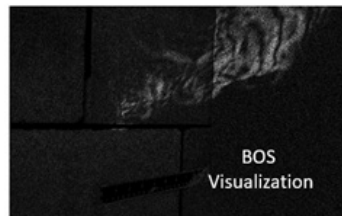
"Building leakage detector using reference-free background oriented schlieren photography," Invention Ref. No. 202205206
US Patent Application 63/345,591 filed March 17, 2023

Unintrusive Building Air Leakage Visualization and Measurement Using Background Oriented Schlieren Photography

Problem: Building leakage accounts for about 4 quadrillion British thermal units of energy consumption in the US and can contribute to poor indoor air quality, occupant comfort, and building material durability. Locating and sealing leakage sites is critical to saving energy and to improving indoor building conditions and durability. State-of-the-art methods involve intrusive blower-door testing and infrared imaging, which require extensive expertise to correctly identify and interpret air leakage sites.

Solution: Background oriented schlieren (BOS) photography detects shifts in background texture to visualize transparent fluid flow in a sequence of images. It requires very small pressure differences between the building and outdoors, so it does not require a blower door and is therefore less intrusive to building occupants, making the technique more adoptable in the market. Since air is visualized directly, there is no risk of incorrectly identifying areas of leakage. Furthermore, BOS can measure the flow rate of individual leakage sites so that leaks can be prioritized during sealing efforts.

Impact: This approach to locating and measuring air leakage in buildings is quicker and less intrusive than current approaches, which is critical to enabling the energy retrofits of millions of existing buildings in the US. New laws will require better than state-of-the-art methods to finding air leakage in buildings. These include New York City Local Law 97, which requires most buildings greater than 25,000 square feet to meet stringent energy efficiency and greenhouse gas emission limits by 2030. The added capability of measuring the flow of individual leaks means that sealing leakage can be prioritized, sealing the biggest leaks first, which ensures buildings meet energy efficiency requirements with reduced time and effort.



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Wellington Muchero

Biosciences Division

Wellington Muchero is a senior staff scientist and geneticist in the Biosciences Division. He leads discovery projects utilizing genome-wide association-mapping studies, quantitative trait loci mapping, and functional validation of genes in eukaryotes. He also leads research to computationally predict and functionally validate conserved protein domains that mediate immune signaling.

Publications

Debjani Pal, Kuntal De, Carly Shanks, Kai Feng, Timothy B. Yates, Jennifer Morrell-Falvey, Russell B. Davidson, Jerry M. Parks, Wellington Muchero. Core cysteine residues in the PAN domain are critical for HGF/c-MET signaling. *Communications Biology*, Nature.

Mutating novel interaction sites in NRP1 reduces SARS-CoV-2 spike protein internalization. Debjani Pal, Kuntal De, Timothy B. Yates, Jaydeep Kolape, Wellington Muchero, *iScience-Cell Press* 2023.

Intellectual Property

"A protein domain modulating host-cell invasion," Invention Ref. No. 202004200 US Patent Application 17/012,139, filed September 4, 2020
European Patent Application 20860537.8, filed September 4, 2020

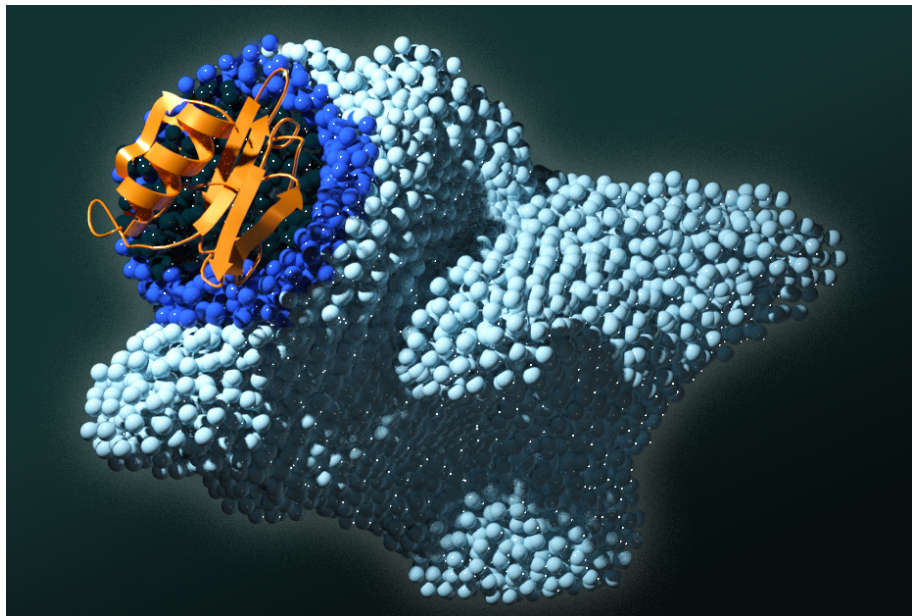
"Modulating protein ubiquitination, cellular internalization and proteolysis," Invention Ref. No. 202205064
US Patent Application 18/323,672, filed May 25, 2023

Methods for Immunoregulation by Modulating Plasminogen-Apple-Nematode Domain (PAN)-containing Proteins

Problem: The immune response of a cell—whether it be human, plant, fungal, or bacterial—is independent of the general immune system of the organism to which the cell belongs. A specific group of proteins—an immunostimulant—increases or enables the ability of a cell to respond to a foreign entity. However, the presence of an immunoregulatory protein suppresses the ability of a cell to respond. Because of this suppression process, cells do not possess the ability to fight against invasive pathogenic fungi or viruses. This process in host cells allows invasive cancer cells to grow without resistance. Recent studies show that inactivation of the PAN domain inhibits interactions with a key receptor in cell development and ultimately blocks cancer progression.

Solution: Inactivation of the immunoregulatory protein in a cell increases the likelihood that the cell can respond to a foreign entity. An ORNL team has developed a method for screening for an immunoregulatory protein, which includes assessing the sequence of a candidate protein to determine if it is an immunoregulatory protein when at least one plasminogen-apple-nematode (PAN) domain with a consensus sequence is found. This method will help in determining a therapeutic compound that can target the PAN domain to inactivate the protein.

Impact: The ORNL team successfully demonstrated that inactivating the PAN domain inhibits spike protein binding in a receptor of the SARS-COV-2 virus. This new screening method provides a way to modulate immune responses in plants and animals. In human cells, this method can be used to inhibit cellular migration in cancer cells and SARS-COV-2 viral spike protein binding. This method could be used in creating genetically modified plants that are resistant to pathogenic infections.



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