Metropolitan Water Reclamation District *of* Greater Chicago

Press Release

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MWRD partners on molecular engineering study to use artificial intelligence and machine learning to detect and remove emerging contaminants from water

Calumet Water Reclamation Plant lab technicians collect and analyze water samples. These findings can help molecular engineers and data analysts study the effectiveness of artificial intelligence and machine learning to address per- and polyfluoroalkyl substances (PFAS) and other contaminants in water.

A new study supported by the Metropolitan Water Reclamation District of Greater Chicago (MWRD) and led by University of Chicago molecular engineers is assessing how sensor-based real-time technology can help detect and remove dangerous contaminants from water.

Growing concern for per- and polyfluoroalkyl substances (PFAS) and other emerging water-contaminating chemicals have given rise to health and environmental concerns and a need for real-time detection to aid wastewater treatment utilities working to address this pollution.

Now scientists from the University of Chicago and Argonne National Laboratory (ANL) working with the MWRD will study the potential of artificial intelligence and organic synthesis to rapidly identify, design and fabricate new chemical probes for sensing and removing thousands of contaminants from water. This innovative platform can assist the water sector encountering these emerging contaminants.

"This partnership will help us get another step closer toward understanding this group of 'forever chemicals' and what we can do to protect public and environmental health from them," said Commissioner Cameron Davis.

According to the United States Environmental Protection Agency (EPA), PFAS are a group of man-made chemicals that includes PFOA, PFOS, GenX, and many other chemicals. PFAS have been manufactured since the 1940s in the U.S. and around the world and used in a variety of industries, in fire-fighting foams and found in many household products, such as stain- and water- repellent fabrics, nonstick products, polishes, waxes, paints, personal care products, and cleaning products.

Over the last decade research has led to the discovery of more than 4,000 different PFAS on the global market. This vast number of PFAS prohibit conventional development of biological or chemical probes for detecting them in water. Current practices to detect and determine the level of these chemicals *(continued)*

are expensive, time-consuming, and require skilled personnel, bulky equipment and advanced analytical chemistry, like liquid chromatography and mass spectrometry, not appropriate for continuous environmental monitoring and management.

Scientists believe by using machine learning to explore the large molecular space of potential PFAS probes, researchers can accelerate discovery and design. The work will also advance data science, simulation and characterization at the U.S. Department of Energy's Advanced Photon Source at ANL. This research also has the potential to help develop new solutions to screening and removing other water contaminants such as pharmaceuticals that can dissolve and slip through treatment processes and harm humans, water quality and aquatic life.

"Precision detection and separation of trace chemicals such as PFAS and pharmaceuticals are crucial for the reuse of reclaimed water to address our global water challenge. Artificial intelligence and machine learning could enable acceleration of the discovery of novel molecular probes toward precision detection and separation," said Dr. Junhong Chen, Ph.D., Crown Family Professor at the University of Chicago Pritzker School of Molecular Engineering and lead water strategist and senior scientist at Argonne National Laboratory.

It was announced recently that the research proposal, entitled "Artificial Intelligence/Machine Learning (AI/ML) Assisted Molecular Engineering to Tackle the Per- and Polyfluoroalkyl Substances (PFAS) Grand Challenge in Water," will be funded by the University of Chicago Center for Data and Computing. The MWRD will collaborate with researchers at the University of Chicago Pritzker School of Molecular Engineering, the University of Chicago Department of Computer Science and ANL, and external partners at the EPA, 3M, Current, AO Smith, and the Air Force Civil Engineering Center.

"We thank our partners at the University of Chicago and ANL for their collaboration on this important research and we look forward to many exciting developments that will safeguard our water environment for generations to come," said President Kari K. Steele.

To learn more about PFAS and emerging contaminants, visit: https://www.epa.gov/pfas/basic- information-pfas.

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