

Agilent Case Study: Agilent Certified Pre-Owned 6470B Triple Quadrupole LC/MS and 1290 Infinity II UHPLC

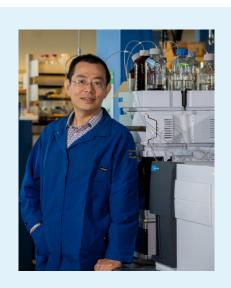
Successful Leadership in Water Pollution Research

Directly dealing with PFAS

Per- and polyfluoroalkyl substances (PFAS) are longlasting synthetic chemicals found in many commonly used products and are persistent within the environment, including our drinking water.¹ The US Environmental Protection Agency (EPA) has identified high concentrations of PFAS as leading to adverse health risks in animals and humans.¹ Therefore, it has become critical for researchers to identify effective methods to remove PFAS chemicals from water sources and destroy them after removal.

Jinyong Liu, PhD, associate professor in the department of Chemical and Environmental Engineering at the University of California, Riverside (UCR), focuses on water pollutant removal and degradation. Specifically, Dr. Liu and the researchers in his laboratory ("Chemistry for the Environment", Liu lab) study ways to break down PFAS and toxic oxyanions such as perchlorate, chlorate, bromate, and nitrate.

Dr. Liu and his team have developed an innovative technology to degrade PFAS chemicals and published a series of papers regarding the structure-reactivity relationship, degradation mechanism and pathways, and performance enhancement in *Environmental Science and Technology and Nature Water*.^{2,3} The team needed to demonstrate that they have the analytical capability to detect PFAS chemicals and their breakdown components in low concentrations to further prove the technology's effectiveness.



Jinyong Liu, PhD

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The Liu lab primarily uses liquid chromatography-mass spectrometry (LC/MS) to identify and quantify PFAS. Jinyu Gao, PhD, is the Liu lab's postdoctoral researcher and a mass spectrometer superuser. Dr. Gao was using an ion-trap mass analyzer for the transformation products analysis but found it challenging to detect low analyte concentrations. Drs. Liu and Gao needed to examine that after treating water with their innovative method, residual PFAS fell below a specific threshold for safe discharge. "For this purpose, we must have a triple quad—and we got this great opportunity to purchase an Agilent product," Dr. Liu said.

An affordable opportunity

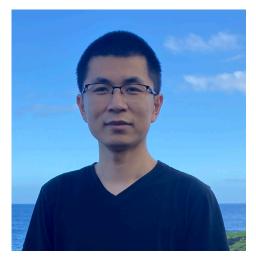
Once he realized their research required a triple quadrupole mass spectrometer, Dr. Liu reached out to three different vendors, including Agilent. But because of the expense, he wondered whether they could fit another mass spec into their budget. "At first, we thought this was not possible," said Dr. Liu. Taking a proactive approach, the Agilent account manager recommended they consider a certified pre-owned instrument and helped them find creative financing solutions.

They evaluated the Agilent Certified Pre-Owned 6470B Triple Quadrupole LC/MS and the Agilent 1290 Infinity II UHPLC. Any internal component that a sample touches within the flow path of an Agilent Certified Pre-Owned instrument is either replaced with new components or rigorously cleaned to pass the same specifications as a new instrument. The certified pre-owned instruments also come with a one-year warranty. During the evaluation, Drs. Liu and Gao mentioned that the Certified Pre-Owned 6470B Triple Quadrupole LC/MS and 1290 Infinity II UHPLC looked and performed like new. In addition, the Agilent representative helped them include an Enhanced Extended Warranty as part of the system cost. Based on their overall evaluation, Dr. Liu had only one remaining question: "Why not?" Because Agilent was able to provide the best offer during the quoting period, find flexible purchasing options, and deliver a warranty to minimize service cost, Dr. Liu and other UCR faculty thought the Agilent system was the best option for their labs, particularly by sharing the financing cost.

Before purchasing their own triple-quad mass spectrometer, Dr. Liu had to budget tens of thousands of dollars each year to cover the cost of sending out samples to a contract lab for assessment. Now they can test on site, reducing their overall operational expenses and demonstrating a positive return on investment.

"For this purpose, we must have a triple quad—and we got this great opportunity to purchase an Agilent product."

Dr. Jinyong Liu
 Associate Professor,
 Department of Chemical and
 Environmental Engineering
 University of California, Riverside



Jinyu Gao, PhD, is the Liu lab's postdoctoral researcher



Successful, low-range detection

The Liu lab has been using the Certified Pre-Owned 6470B LC/TQ and 1290 UHPLC since May 2023, and has achieved the desired sensitivity in detecting trace amounts of PFAS. In 2022, the EPA proposed a PFAS limit of 0.004 ng/L (4 x 10^{-6} ppb, 0.004 ppt); but many scientists found this level could not be effectively measured. In 2023, the EPA proposed a limit of 4 ng/L (0.004 ppb, 4 ppt), as measured via the EPA1633 method.⁴ By using the 6470B LC/TQ, Dr. Gao has been able to detect a wide variety of PFAS structures with detection limits as low as 50 ng/L (0.05 ppb, 50 ppt) to 1,000 ng/L(1 ppb, 1000 ppt). With the Certified Pre-Owned system from Agilent and a rapid solid phase extraction (required to prevent unwanted species from entering the system while concentrating the target PFAS), Dr. Liu and Dr. Gao can now readily detect PFAS in the concentration range of the current EPA requirements.

Although the EPA may not currently require detection thresholds to be as low as 4 ng/L, Drs. Liu and Gao anticipate that could change in the future. They also anticipate that the EPA will want to assess more PFAS structures than they currently do today. Preferring to be ahead of the EPA's requirements, the Liu lab has already demonstrated the capability to identify novel PFAS structures at low detection limits.

In their 2022 publication, Dr. Liu, and another PhD student (Dr. Zekun Liu), illustrated how their optimized UV/sulfite and iodide (UV/S + I) system removed more than 99.7% of perfluorosulfonates (PFSAs) and perfluorocarboxylates (PFCAs), and more than 90% of concentrated PFAS mixture from synthetic wastewater.² Results like this place the Liu lab at the frontier of PFAS research.⁵⁻⁹ "We have already established a very strong capability in environmental chemistry and pollutant degradation. I can say we're leading the field in understanding how PFAS degrades and knowing how to achieve deeper degradation," Dr. Liu said.

Partnership and education

With such strong scientific leadership in PFAS research, it isn't surprising that Dr. Liu has formed partnerships with members of industry. While most of their experimentation in the past was benchtop research using synthetic water samples, Dr. Liu, Dr. Gao, and another postdoctoral researcher, Dr. Dandan Rao, have started evaluating real-world water samples from industry partners.

The university lab has collaborated with environmental, engineering, and construction firms innovating in fields such as water resource management and engineering, water pollution, and climate change. These collaborators send challenging wastewater samples from groundwater remediation systems such as ion-exchange and foam fractionation to the Liu lab for PFAS degradation and analysis. In the future, as they work with more industry partners, Dr. Liu and his lab members expect their service-based testing to increase.

Throughout their experimentation, Dr. Liu and his colleagues have noticed how useful it would be for their lab members to obtain hands-on experience using mass spectrometers. For their graduate students to compete in the job market, practical knowledge of running various mass spectrometers would be ideal. Dr. Liu envisions his lab becoming a training center for PhD students to learn and use mass spectrometry to help their career preparation and development.

Conclusion

For the future of their significant environmental research, it was important that Dr. Liu and his colleagues obtain the right instrumentation for the laboratory. Although at first it seemed as though they would be unable to afford triple quad mass spec, Agilent representatives found a creative and effective solution with a Certified Pre-Owned 6470B LC/TQ and 1290 UHPLC. Now Dr. Liu and his lab members can continue their influential work, helping to improve our environment's water quality, and bring great science to life.



References

- US EPA, O. A. PFAS Explained. 2016, https://www.epa.gov/ pfas/pfas-explained (accessed 2023-09-18).
- Liu, Z.; Chen, Z.; Gao, J.; Yu, Y.; Men, Y.; Gu, C.; Liu, J. Accelerated Degradation of Perfluorosulfonates and Perfluorocarboxylates by UV/Sulfite + Iodide: Reaction Mechanisms and System Efficiencies. *Environ. Sci. Technol.* 2022, 56 (6), 3699–3709. https://doi.org/10.1021/acs.est.1c07608.
- 3. Gao, J.; Liu, Z.; Chen, Z.; Rao, D.; Che, S.; Gu, C.; Men, Y.; Huang, J.; Liu, J. Photochemical Degradation Pathways and Near-Complete Defluorination of Chlorinated Polyfluoroalkyl Substances. *Nat Water* **2023**, *1* (4), 381–390. https://doi.org/10.1038/s44221-023-00046-z.
- Surface Water. Analysis of per- and polyfluoroalkyl substances (PFAS) in aqueous, solid, biosolids, and tissue samples by LC-MS/MS. Epa.gov. https://www.epa.gov/system/ files/documents/2022-12/3rd%20Draft%20Method%20 1633%20December%202022%2012-20-22_508.pdf (accessed 2023-10-23).
- Gao, J.; Liu, Z.; Bentel, M. J.; Yu, Y.; Men, Y.; Liu, J. Defluorination of Omega-Hydroperfluorocarboxylates (ω-HPFCAs): Distinct Reactivities from Perfluoro and Fluorotelomeric Carboxylates. *Environ. Sci. Technol.* 2021, 55 (20), 14146–14155. https://doi.org/10.1021/acs. est.1c04429.

- Liu, Z.; Bentel, M. J.; Yu, Y.; Ren, C.; Gao, J.; Pulikkal, V. F.; Sun, M.; Men, Y.; Liu, J. Near-Quantitative Defluorination of Perfluorinated and Fluorotelomer Carboxylates and Sulfonates with Integrated Oxidation and Reduction. *Environ. Sci. Technol.* 2021, 55 (10), 7052–7062. https://doi.org/10.1021/acs.est.1c00353.
- Bentel, M. J.; Liu, Z.; Yu, Y.; Gao, J.; Men, Y.; Liu, J. Enhanced Degradation of Perfluorocarboxylic Acids (PFCAs) by UV/Sulfite Treatment: Reaction Mechanisms and System Efficiencies at PH 12. Environ. Sci. Technol. Lett. 2020, 7 (5), 351–357. https://doi.org/10.1021/acs.estlett.0c00236.
- Bentel, M. J.; Yu, Y.; Xu, L.; Kwon, H.; Li, Z.; Wong, B. M.; Men, Y.; Liu, J. Degradation of Perfluoroalkyl Ether Carboxylic Acids with Hydrated Electrons: Structure—Reactivity Relationships and Environmental Implications. *Environ. Sci. Technol.* 2020, *54* (4), 2489–2499. https://doi.org/10.1021/acs.est.9b05869.
- Bentel, M. J.; Yu, Y.; Xu, L.; Li, Z.; Wong, B. M.; Men, Y.; Liu, J. Defluorination of Per- and Polyfluoroalkyl Substances (PFASs) with Hydrated Electrons: Structural Dependence and Implications to PFAS Remediation and Management. *Environ.* Sci. Technol. 2019, 53 (7), 3718–3728. https://doi.org/10.1021/acs.est.8b06648.

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