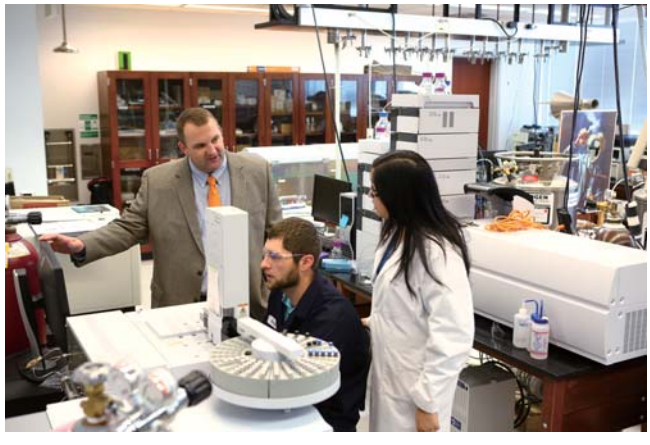
# Interview with Prof. Kevin A. Schug

We interviewed with Dr. Kevin A. Schug, Associate Professor and Shimadzu Distinguished Professor of Analytical Chemistry in the Department of Chemistry and Biochemistry at the University of Texas at Arlington (UT Arlington). His research is mainly on the separation of bioactive chemical compounds with mass spectrometry techniques. Also, he is currently undertaking one of the most extensive investigations of the potential impact of industrial processes, such as unconventional drilling and hydraulic fracturing, on our environment. He and Shimadzu started collaborative work in 2012 when the Shimadzu Center for Advanced Analytical Chemistry was established.

**Dr. Schug, we greatly appreciate you taking time to talk with us.**
**At first, could you tell us the background of this collaborative research? Why did you choose Shimadzu as your partner?**

First, thank you for this opportunity to speak with you. It has been a real pleasure to work with Shimadzu, and I sincerely appreciate your efforts to tell our story. My interactions with Shimadzu actually began way back in 2000, when I was a graduate student at Virginia Tech. Our analytical group, headed by Prof. Harold McNair, regularly administered American Chemical Society short courses in gas chromatography, liquid chromatography, sample preparation, and other topics. Shimadzu was always willing to put instruments on site for these courses, and I was able to build a good relationship with a number of their technical and sales employees. In the end, I completed my dissertation research on the topic of adduct ion formation in electrospray ionization, using a Shimadzu QP8000α single quadrupole mass analyzer.
After my post-doctoral stay at the University of Vienna, I joined the faculty in the Department of Chemistry and Biochemistry at U.T. Arlington. Within a year or two, contact was made back to Shimadzu, and we were able to organize the acquisition of an LCMS-ITTOF, in 2007, through the Shimadzu Equipment Grants for Research Program. It was only one of a handful of such systems available in the country at that time, so we had a unique opportunity to perform cutting edge research that others could not, based on the powerful features of the instrument. Not long after that, we began discussions of a larger partnership. Much of the success of establishing what would ultimately be the Shimadzu Center for Advanced Analytical Chemistry and the Shimadzu Institute for Research Technologies at U.T. Arlington was due to our forward looking administration. It became quickly clear to those involved, that this partnership would be a big win for all involved. U.T. Arlington would acquire a wide range of state-of-the-art instrumentation. Shimadzu would gain an active partner performing cutting edge research using their instrumentation. My laboratory could expand into a variety of different areas where some opportunities for research were present – namely, in trace analysis of compounds from biological fluids, using CoSense and triple quadrupole mass spectrometry, and into assessing the potential environmental impact of unconventional natural gas and oil processes, using a wide range of instrumentation. Clearly, one of the main reasons why our partnership has been successful is due to the personal relationships and support provided.



**Then could you outline the research and let us know what discovery and achievement have been made so far?**

Our research on trace quantitative analysis from biological fluids began through a collaboration with a local medical school, where they were piloting the clinical use of estrogens for the treatment of traumatic brain injury. They could use an immunoassay to quantify the level of estrogens in plasma, but no such validated method existed for trace quantification of estrogens in cerebrospinal fluid. We began with a traditional liquid-liquid extraction off-line sample preparation technique, but learned quickly that the workflow took too long to effectively handle a large number of samples. At that time, we were introduced to Shimadzu CoSense, which features the use of restricted access media for on-line sample preparation. We assembled the set-up in the lab with the help of Shimadzu personnel and set about developing more efficient methods. We have been successful in developing ultra-sensitive methods (low parts-per-trillion detection limits) for detection of estrogens in cerebrospinal fluid and in plasma. We have also carried out some fundamental studies on how best to optimize trapping efficiency on the MAYI trap restricted access media offered by Shimadzu.
Our research on groundwater quality is unique. By this point, we have taken and analyzed over 800 well water samples in proximity to unconventional drilling and hydraulic fracturing activities. This is the largest effort to date of this kind. In 2011, we realized that very little work had been done to assess potential environmental impacts of this industrial activity, which has been so very important to the United States economy. It has been our goal to be objective and simply collect data that no one else was collecting. As an academic entity, we could remain wholly unbiased, and in fact we have done much of our work without outside support, beyond some funds provided by the University, and the availability of a large suite of analytical instruments based on the Shimadzu partnership. We have developed a core set of analytical techniques based on Shimadzu GC-MS, headspace GC-FID/BID, ICP-OES, and TOC/TN analyses. These methods borrow best practices from standard methods, but also build in a combination of targeted and untargeted strategies to allow for a comprehensive evaluation of water quality. In an early

report, we found evidence for indirect impact of unconventional drilling processes on water quality in North Texas. We are currently working on two manuscripts that report a survey of a larger section of North Texas, and a time-course study where samples were taken before, during, and after drilling activity in west Texas. We expect that these studies will bring vast new insights into the relationship between modern gas and oil extraction, and its potential environmental impact.

### Why are you interested in this research? What is the goal?

We are driven by the interest and desire to find new solutions to challenging analytical problems. We also want this effort to involve high impact problems. The clinical world brings significant analytical challenges, and it involves issues relevant to human health. Environmental analysis is not something I would have pictured our group doing five years ago, but it has now become a major research effort for us. Just like clinical work, there are real human impacts to environmental issues, and the work we are doing on groundwater quality brings us close together with individuals and their homes. The goal in that effort is to assess whether there are any deleterious effects of current practices of unconventional oil and gas extraction. As this is research that very few people are pursuing, it is that much more important to dedicate the time and resources to it. It is rewarding to work in areas that can make a difference, as well as provide optimal training for students so that they can carry the banner forward.

### How are our instruments helping you?

We could not do any of this work without our Shimadzu instruments. Not only that, the unique high performance features of many of the systems we use enable us to do some things that would be very difficult for others. I have always felt that Shimadzu was smart in the lines of instrumentation they develop. It is clear that you are not trying to fit completely in existing markets, but rather to set new markets with specialized instruments and solutions. For our pre-clinical and clinical work, we use the CoSense system coupled to highly sensitive triple quadrupole mass spectrometry. Only a few other manufacturers offer similar configurations, and thus, we can be quite unique in the methods that we develop; those methods also provide superior performance. For the groundwater work, we use a very diverse group of instruments. The fact that Shimadzu provides so many different choices gives us some flexibility to ensure that we can get the job done right and see the things we need to see in order to make reliable conclusions.

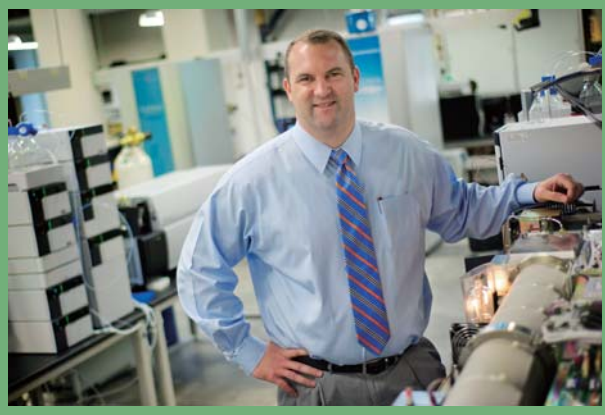
### What are Shimadzu's strengths compared to other vendors (not limited to the instruments)?

I have always said that Shimadzu's greatest strength is its people and service. I have been in the role of a customer for Shimadzu and for many other companies, and I have always found that Shimadzu service has been the most helpful and reliable. I like the idea that I do not necessarily have to have a service person on site to get help with a problem. Oftentimes, a phone call yields a simple fix that we can quickly and inexpensively implement. Now that we are part of a larger partnership, we enjoy a much closer interaction with Shimadzu. This means that our students have regular contact with engineers, applications chemists, and sales/marketing personnel to get more out of their education. In a similar fashion, we get to work together many times on projects of mutual benefit. I am happy to say that I have had, and I am sure will continue to have, very productive collaborations with Shimadzu Scientific Instruments in the United States and Shimadzu Corporation in Japan. I am even looking forward to future partnerships with other Shimadzu subsidiaries around other parts of the world. I could not imagine a better relationship to help enable my research, that of others at U.T. Arlington, and advance the education of our students in ways virtually impossible at other institutions.

### Finally, could you share any requests that you have with respect to analytical and measuring instrument vendors?

Keep doing what you are doing. Keep innovating. And, selfishly, keep us informed about the newest releases and solutions. I am always amazed at how you are constantly releasing new technology into the marketplace. Through the Shimadzu – U.T. Arlington partnership, we have remained on the cutting edge of research in analytical chemistry, and that is a very important place for us to be, as we continue to move towards Tier One research status. We have several instruments that are largely unique in North America. We appreciate the receptiveness that Shimadzu has had to our suggestions for new products and improvements to existing ones. Ultimately, not everyone needs exactly the same solution, and it is important to be able to work together with a vendor and partner who is willing to be flexible to help us achieve our goals. Thank you! I look forward to a rewarding and productive future in our continuing interactions.

### It was significant to know what you think about us and our collaboration. We will strive to meet your request more than ever. Thank you very much.



His recent publications: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2. Schug, K.A.; Sawicki, I.; Carlton Jr., D.D.; Fan, H.; McNair, H.M.; Nimmo, J.P.; Kroll, P.; Smuts, J.; Walsh, P.; Harrison, D. A Vacuum Ultraviolet Detector for Gas Chromatography. Anal. Chem. 2014, 86, 8329-8335.

3. Papouskova, B.; Fan, H.; Lemr, K.; Schug, K.A. Aspects of Trapping Efficiency And Matrix Effects in Development of a Restricted Access Media-Based Trap-and-Elute Liquid Chromatography-Mass Spectrometry Method. J. Sep. Sci. 2014, 37, 2192-2199.

4. Fan, H.; Papouskova, B.; Lemr, K.; Wigginton, J.G.; Schug, K.A. Bulk Derivatization and Direct Injection of Human Cerebrospinal Fluid for Trace Level Quantification of Endogenous Estrogens Using Trap-and-Elute LC-MS/MS. J. Sep. Sci. 2014, 37, 2010-2017.

5. Barnes, J.S.; Schug, K.A. Oxidative Degradation of Quercetin with Hydrogen Peroxide Using Continuous Flow Kinetic Electrospray ・Ion Trap ・Time of Flight Mass Spectrometry. J. Agric. Food Chem. 2014, 62, 4322-4331.

6. Nguyen, H.P.; Chandel, N.S.; DeBerardinis, R.J.; Schug, K.A. Hydrophilic interaction liquid chromatography ・tandem mass spectrometry to detect and quantify dicarboxyethyl glutathione, a metabolic biomarker of fumarate hydratase-deficient cancer cell. J. Sep. Sci. 2013, 36, 3303-3309.

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9. Yang, S.H.; Wang, E.H.; Gurak, J.A.; Bhawal, S.; Deshmukh, R.; Wijeratne, A.B.; Edwards, B.L.; Foss Jr., F.W.; Timmons, R.B.; Schug, K.A. Affinity Mesh Screen Materials for Selective Extraction and Analysis of Antibiotics using Transmission Mode Desorption Electrospray Ionization Mass Spectrometry. Langmuir 2013, 29, 8046-8053.

10. Tedmon, L.; Barnes, J.S.; Nguyen, H.P.; Schug, K.A. Differentiating Isobaric Steroid Hormone Metabolites Using Multi-Stage Tandem Mass Spectrometry. J. Am. Soc. Mass Spectrom. 2013, 24, 399-409.