

## Seeking Clarity: A Conversation with Dr. Imma Ferrer and Dr. Michael Thurman of CEMS

Amid today's perfect storm of global pressures – climate change, population growth, urban expansion, dwindling resources, greenhouse emissions, and many more – the idea of "saving the environment" can take on countless meanings. Still, no matter how it is defined, the phrase has never had greater prominence in our shared consciousness – or a greater sense of urgency.

Indeed, no matter where you look, there's "saving the environment" work to be done – but where to start? For Drs. Imma Ferrer and Michael Thurman, the answer was as clear as the water flowing in the mountain streams of the Colorado high country. Both scientists can be found at the Center for Environmental Mass Spectrometry (CEMS) at the University of Colorado at Boulder, where they work to develop new methods for environmental water chemistry analysis. The focus of CEMS – namely, "the detection of pharmaceuticals, hormones, and other organic contaminants in water and evaluating the effectiveness of methods for removing these compounds" – strikes directly to the heart of their passion for understanding the anthropogenic impact on environmental water quality.

Agilent spoke with this dynamic duo – who, in addition to being partners in science, are also partners in their life outside the lab – about how technological advancements are impacting their work, and how their work in turn is influencing the way important questions get answered.



Imma Ferrer, PhD

Research Scientist  
University of Colorado, CEMS  
USA



Michael Thurman, PhD

Research Scientist  
University of Colorado, CEMS  
USA

**Agilent:** What inspired you to get into science?

**Dr. Thurman:** "I grew up during the space race, at a time when science was important, and scientists were important people. Combining those early impressions of science with my love of the outdoors led me pretty naturally to a PhD in geochemistry."

**Dr. Ferrer:** "My path was different. I grew up in a huge city where I was mainly exposed to science in school. It always interested me, and I was lucky to have some very good teachers, especially in college. Also, one of my older sisters became a chemist, so that inspired me to follow in her footsteps."

**Agilent:** How would you describe the partnership with Agilent, who provides analytical instrumentation for your lab?

**Dr. Thurman:** "A colleague suggested the idea of pursuing a formal collaboration with Agilent in 2003. I thought it was a great idea, because by that time, we had already been collaborating with them informally for years, as I got my first Hewlett Packard mass spec in 1985 and Imma got a single quad in 1998."

**Dr. Ferrer:** "Over the last 10 years or so, Agilent has placed instruments in our lab as part of our formal collaboration and replaced them as new models were introduced. We have also had access to service and support, but the instruments are so robust there's been very little need for it."

**Agilent:** What are some of the challenges you've faced over the years?

**Dr. Ferrer:** "In the beginning, people would come to us and say, 'Tell us as much as you can about what's in this water sample.' So, the challenge was to narrow down what compounds were important and relevant to them, and of course to figure out what compounds we could actually see."

**Dr. Thurman:** "In 2004, benchtop accurate mass was just starting, and there really weren't any tools to go with the instrument – the software was just beginning to be developed. We did a lot of pioneering work in that area, including a patent with Agilent on isotope spacing, and we've also authored or co-authored maybe 30 or so Agilent application notes. Today, there are powerful tools in the software, but we've also developed our own style, our own approach, and it seems the software has in many ways developed along with that."

"Now our challenge is 'Big Data'. The instruments can generate so much information, but what do we do with it?"

**Dr. Ferrer:** "From the moment a sample enters our lab, we can run it within a day. But we can spend weeks or months extracting data from that single sample. Software becomes a very important part of the process."

**Agilent:** You're using Agilent MassHunter Explorer software, which combines data extraction, analysis, and identification features into one streamlined tool for generating critical insights. How has that figured into your work?

**Dr. Ferrer:** "Before, we had to focus on the individual samples; MassHunter Explorer software allows us to pull back and see everything at once. We can start to see connections we might not have seen by looking at each sample individually."

**Dr. Thurman:** "It allows us to quickly move from individual samples to the big picture. It lets us see this huge amount of data in context, so we can make choices that get us to the answer as fast as possible. That helps our work be relevant, because people are anxious to know things – they don't want you to say 'Well, in a year or two we will have an answer for you.'"

Imma does an interesting thing: she archives many of our extracts in the freezer for later reanalysis. We can go back and look at old samples with new software, and that's been very powerful. Not only can we look at retrospectively look at data files, we can also retrospectively look at the samples themselves as new tools like MassHunter Explorer become available."

**Dr. Ferrer:** "A given sample may have thousands or even ten thousand 'features', as they're called. But some of those are background ions that are always there, so you have to narrow it down to what's important. The software helps us quickly focus on a relatively much smaller number of compounds that are of particular interest."

**Dr. Thurman:** "The software also allows us to do something that we intuitively know, but it's nice to be able to show it with data. For example, we know which samples are the

'natural' samples that don't have contaminants, and we have an idea about which samples are contaminated. This software helps us show data to confirm these intuitive hypotheses that we know from the sampling and the geology. The software gives us the ability to pull these apart; there are various statistical packages that help us determine significance. Then we can do a deep dive into those samples."

**Dr. Ferrer:** "Previously, this kind of analysis involved a lot of what we called 'peak clicking'. It worked, but answers were slow in coming, and it was difficult to catch everything."

**Dr. Thurman:** "Twenty-five years ago, really all we could do was targeted analysis. You had standards, you ran samples, you looked for specific compounds. Today, if a lab isn't doing accurate mass analysis with these kinds of software tools, they're at a real disadvantage."

**Agilent:** In what ways has MassHunter Explorer met or even exceeded your expectations?

**Dr. Ferrer:** "I think we've gotten more than we expected. Before, we would run samples, analyze the data, then write a paper. Now, there are so many interesting outcomes to share, we have papers lined up waiting to be written."

**Dr. Thurman:** "I can give you an idea how exciting it can be. When Mt. St. Helens erupted, a colleague collected samples there and freeze dried them. About a year ago we analyzed some of those samples, and we found some of the same compounds we find among contaminants from house fires. Suddenly, there are all these compounds and isomers that you had no clue were there, showing you connections you never expected. It's this kind of excitement that can take you off on a tangent that sometimes keeps you from keeping up with the writing."

**Agilent:** What inspires you now?

**Dr. Ferrer:** "The new tools that are available today are bringing such great insights, we're finally able to start asking big questions about things like health and preserving the environment, rather than just focusing on finding out which individual compounds might be present."

**Dr. Thurman:** "We are at a point where we're generating interesting results that can start to answer these important questions, but there is so much data out there, and so many papers, that it might be difficult to be heard above the noise. Industry collaborations, like ours with Agilent, give us new opportunities to meet people and exchange ideas and expertise. These are conversations that can take us in directions we may never have expected."

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