Interview with Nelson Vinueza

Laura Dyster: Welcome to the Biocolours2024 conference podcast, where you get a glimpse of the upcoming conference next June. My name is Laura Dyster, and I am part of the conference organizing team. Our next speaker here is Associate Professor Nelson Vinueza, who will be one of the session keynote speakers at the conference. Welcome, Nelson.

Nelson Vinueza: Well, thank you for having me. And I'm glad to be here.

LD: I'm happy that you accepted our invitation to be one of the session keynote speakers. And we're looking forward to hear you talk more in depth about your field. But today, we're going to talk briefly about your career and what your research focus has been.

NV: That's great.

LD: At the beginning, can you provide an overview of your background and especially your experience in mass spectrometry and how the context of dye characterization and analysis is involved?

NV: Sure. So as you mentioned earlier, I'm an associate professor in the Department of Textile Engineering, Chemistry and Science. at the Department of the Wilson College of Textiles and the Department of Chemistry at North Carolina State University. I joined NC State in August 2013 as part of the Chancellor's Faculty Excellence Program. Since then, I have been the Max Weaver Dye Library Director, which is historically a collection of 100,000 synthetic dyes. And in 2010, when I was pursuing my postdoctoral work, I was part of this Center of Direct Catalysis Conversion of Biomass Available Fuels at Purdue University, where in the same university, I earned my PhD with Professor Hilkka Kenttämaa, which is Finnish, so that makes a big connection for me going over there. And my areas of research sometimes have around three aspects of mass spectrometry. One's fundamentals, the other's instrumentation and applications in dye, textiles, forensics and biofuels. And basically that's what we do. So one of the things we do with mass spectrometry, we can do a lot of characterization and dyes is becoming a big field in my research portfolio.

LD: Could you tell us more about the Max Weaver Dye Library and its significance in your research?

NV: Sure. You know, one of the big things about this collection of library is, first of all, it's a work, tremendous amount of work of people from Eastman Kodak at that time. So we have dyes from the 1950s to the 1990s. So this had been all synthetic dyes that have work that a group of scientists have synthesized them and see different properties of dyes. So in 2014 I arrived to the Wilson College of Textiles, where one of the reasons I'm in the college is this collection. So this was a way to get more in the fundamentals, how dye works, and expand my area of mass spectrometry, just focusing more on dyes. Because with that big collection, you know, we can learn more how a dye fragments on the mass spectrometer and also start learning more about properties of dye that in some cases have not been seen by the public eye. So there's a lot of things, maybe there's some dyes that have been patented, but there's a lot of very, you know, big number of dyes that have not been still tested. And that's one of the things we are doing at this point, that we are expanding the Max Weaver Dye Library in the use of these dyes in completely different areas, like medicine, creating new type of solar cells, I would say energy in that case, energy conversion. The other, what we're trying to do is more sustainable dyes, you know, kind of helping to see what part of the dyes can be changed or so. So, it's a great collection. We have something that someone else have worked on it, and we are using this tremendous treasure trove in our path to make these great organic molecules more useful than just giving color.

LD: So how did the idea of creating a dye database come about?

NV: This is very simple. So if you think about 100,000 dyes, you say how I can see this. So we have a specific location in the Wilson College of Textile. So it's a shelves with drawers and when you open a drawer, you have each row we have depending on the drawer between 600 and 1000 dyes. So when you open, it's very hard to see which dye you want. So one of the things we try to see is if we can start digitalizing the library and create a database that now with machine learning, we can start doing kind of more specific type of searches, like, for example, if you have a dye that has certain characteristics for a fabric or for a specific test, like, you know, a sensor, can we search a similar dye in the database? So, our idea and our original paper came out in 2017 in Chemical Sciences and Open Source. Probably I will show something of that in the conference. But that was a way to show how a small amount of dyes that we can digitalize at the time, there was around 2700 dyes that we did chemoinformatics. So learn about what all these structures can be and can do. And one of the biggest things that we learned is how unique these dyes can be. So one of our collaborators, Anthony Williams, which was the original creator of ChemSpider, this huge website of, you know, you can find structures and information about any chemicals. He made a comparison of 150 structures of the digitalized library we have at that time that we decided to give to the public, to the scientific world, to see what's the value of the library, and compare those 150 with, at that time, 58 million structures present in ChemSpider. What was so surprising for us was that 143 dyes of the universe of 150 we give to the scientific community were unique and were not in ChemSpider. Only seven appear. So when this happens, we were like, wow, it's like we have like, you know, a lottery ticket. And that

shows that that potential of the library. So one of the things with this is we can start applying this type of concepts of having these molecules, because the nice thing about dyes is they have color, but they have properties. And we can start seeing if these molecules can be used in different fields. So, a database can always help to understand more structure relationship, structure color relationships, or interaction between other molecules or proteins or any type of, you know, interaction between two different chemical entities. That's what I can say.

LD: Well, it's such a vast collection of synthetic dyes, so you must have encountered some challenges while working with it.

NV: Of course. One of the things is our digitalization has to be manual. And this is for a big reason. I'm not sure if it's going to show in the video, but in my background, probably you can see how some of the vials look like on that sense. But the structures of the vials that are in the collection, they're handwritten. And since our vials are similar to a test tube, so it's very hard to find an optical device that can read and actually extract the chemical structure from it. We have tried to see some collaboration with people that work on this area, and it's really hard. So we start finding ways to do it, but one of the big challenges for us is enter each dye manually. So we have a great group of students that it's a, you know, we have undergrads that help us with that. We're following with grad students in my lab that have done it. And we are in collaboration with other universities helping us in this effort and try to see how we can do this a little bit more automatic. But that's kind of one of the biggest challenges. The other challenges that we find in here is when, you know, someone wants a dye that we have selected for a certain study, we have to provide them with a quality control. So, normally I use mass spectrometry to do that. So, sometimes we can check if some of the dyes are good for testing, right, or not. And this sometimes can be, you know, most of it has been very positive for us because a lot of the dyes have not been degraded for what we have seen, but overall, it's more positive to give our collaborators, you know, three to five milligrams of the dye for testing and finding those results and say, hey, this works for us. So, I would say that's kind of the most challenging parts that we have. Digitalization and make sure the dyes are still good and some not degraded. We have found some, but still the numbers are pretty low still on the degradation side, but still we take care of the library too.

LD: So you use mass spectrometry for dye characterization.

NV: Yes.

LD: So what are the key aspects that you focus on in the characterization of dyes and their degradation products?

NV: Yeah, so that's a really good question. One of the things about dyes that intrigue me the most when I start to work with mass spectrometry is, there's a great science about how these dyes can consider an automatic system. But what you see sometimes in textbooks where people have studied, there are sometimes very limited structures that people have seen. So having a collection of 100,000 gives you an idea of a study how a simple change of a functional group can make the molecule different behavior in the mass spec and how fragments differently or so. So, one of the things we start finding in dyes is, first of all, the structure sometimes are not correct based on the public knowledge. A lot of the dyes that are, especially the new dyes, are patented protected. So, it's very hard to determine what the structure is, but the ones that are out there, I can tell you one of the things we have done with high-resolution mass spectrometry is, sometimes we have a group of commercial dyes we check just for quality control, and we have detected 70 percent of the structures that are written on literature or have been public match what we see, and 30 percent not. And this can be small changes on the manufacturer, but they are not representative of what the structure should be. So, in this case, mass spec is given as a better idea if we have the dye or not. And that other aspect is when there's a part of mass spectrometry called tandem mass spectrometry, which means, it's an experiment we do in our machine that in easy terms you have a molecule that we are going to make it fragment when it hits a targeted gas. It can be nitrogen, it can be argon. So these fragments are related to the structure. So sometimes when we have an unknown, we try to work with tandem mass spectrometry and try to determine how this molecule breaks apart and that helps to build up an unknown structure. And this is key, especially when we start entering the field of how a dye degrades. So one of the things we had to learn about dyes is, depending on the type of material you have, there's probably a different dye. So if we talk about simply aspects of disperse, dyes that are more for synthetics, acid, or reactive. Reactive dyes are already known to be in cotton. You see acids normally you see in nylon, a lot of nylon, you can see those. So which material it is, it's a dye. So depending on that, maybe we have to have a lot of conditions with mass spectrometry, one of the things we had to think if you think in the broader aspect, mass spectrometry is three parts. First, the ionization, how I charge the molecule to see it. The other is the mass analyzer, that's where I'm going to separate any ions or interferons, and I'm going to detect them later.

So ionization is the heart of the mass spectrometry, because if it's not charged, I cannot see anything, I cannot manipulate nothing in the mass spectrometer. So some of these dyes, especially disperse are more usually in synthetic dyes, are not charged. So electrospray ionization has worked really well, almost with every dye. However, we find that atmospheric photoionization can be more useful in determining some things with dispersed dyes. So once we charge the molecule, there's a good study to understand how these dyes behave under ionization conditions. Once we charge it, we see it on the mass spec, we get something about the structure, and, you know, determine if what we are seeing on the flask

or in the vial is correct. Now, imagine now this dye goes through a process of biodegradability, goes to a landfill. You know, we have done a study with cotton fabrics that are being simulated in landfills. So the cotton is going to degrade, but sometimes the reactive dye that's there is not. So we have to find ways to see what happened with the dye structure. And because there's a low quantity of material, about mass spectrometry is key on it. So we don't need too much, you know, amount of material to do our test. Basically, I can do a test on three milligrams of fabric. If you take into account that normally a 3% of weight of fabric is the dye, in 3 milligrams, that's what I can see very easily and do tests. So in that way, we have learned about, especially in landfills, how dyes degrade. In this case, what we have found, dyes that have, that being polar, have sulfonate groups, for example, that sulfonate group is gone. And, you know, it is more hydrophobic, so it's more hydrophobic and bioaccumulate. And so we are finding in our study shows that in this case, mass spectrometry is very helpful in determining the degradative products, these derivatives that come from the main structure. So our group has become an expert on this field, and we have done this work since 2015. And we are transitioning to different dyes because each dye has their own structures. Even if we think about in the market, 80% are azo dyes, 80 to 85% are azo dyes and 50% are entrepreneurs and the rest are the 5%. But even this having different azos is challenging or different entrepreneurs challenge to see what they are because there's not really a lot of information about the structure if they're still patent protected.

LD: So you have developed specific methods for the dye analysis?

NV: Yes, so there's ways to do it. We can use HPLC to separate if we take the dye out from a, we call it matrix, can be the fiber of the soil, where it has been, or the water system. And when we have done that, our idea is to see what is in there. So we have learned and created methodologies that allow us to do a faster screening, to learn where we can have a potential candidate of degradation. And they've worked backwards, you know, like a like a retroengineering to see, okay, we have find this where it can come from. So that's what we have done. And we have an expertise on it. And we use a couple of mass spectrometer. One is a portable time of flight. The other is a linear trap. And also we have orbit traps that can be helpful for us. And we're going to start working with ion mobility mass spectrometry too in the coming future.

LD: So these methods that you have developed really enhance our understanding of the dye structures and behaviors.

NV: Correct. So sometimes, you know, sometimes we want to sew, it's very hard to, if you think about, I can give you an example with disperse dyes. So disperse dyes, since they are in the fabric, they are not like a reactant that covalently bond to the fabric. You know, you

can with a solvent, you can easily extract it and try to test it, right? So doing this traction and everything, there's possibilities that you can lose some of the material. It means you're talking about degradation products. We have technology and we have a station called direct analysis in real time called DART. And that we hooked up with the mass spectrometer is we can put the fabric directly in front of this DART and the DART will have a hot helium, metastable helium go through it and dissolve the dyes from the fabric directly to the mass spec. So this way we don't lose material and we don't lose anything that an extraction can happen. So first of all, we speed up the process to get a general idea of what's going on and give us the the certain that we are getting all the things coming out from the fabric. And we're talking about fiber of, you know, between one millimeter or less, or it can be, you know, a thread for us is a lot of material that we can use on this technology. So it can be very helpful for us.

LD: Yeah, thank you. And I'm sure that research is, of course, a lot of it is done by one person or one team by themselves, but I'm sure that collaboration with other researchers and institutions play also a major part in your research.

NV: Correct. So, you know, I'm a big believer of especially multidisciplinary collaborations because nowadays everyone cannot be an expert, right? We can, as an individual, I cannot be an expert in everything. So it's good to establish collaborations that, you know, work on different areas or different aspects, like, for example, in dyes, and merge them together and see how we find some common ground to collaborate. But not more important than that is I will learn something from that group or that group of people, and they will learn something from my lab. So I think one of the great things that I have been in academia these years, it's almost 10 years, looks like a long time already. I have got great collaborations over time. And not only the science have a higher impact, but these teams become like families in many ways. We have close connections. So I think the work and collaboration we see in Finland are going to be great for us in the future. So I always think that always someone from different perspectives can add that, you know, diversity, not only on the, you know, I would say on the aspect of background, but I would say over the way of how we troubleshoot problems can be very helpful. And I think I learned that when I was working on the biofuel project, when I was doing my postdoc, when, you know, me as a chemist, I had to work with biologists, people from chemical engineering, and mechanical engineering, and people that works also in genetics. So, it was a big effort to understand how biofuels and how we can tailor biofuel for our purposes. So, that really showed me how getting people from different backgrounds can really have more high impact work, but also kind of learn more about, you know, explore things that kind of are blind to our eyes, because we are not in the field. So yeah, I think that's the great thing about collaborations, is nothing we can compare to anything else.

LD: Yeah. Thank you. So what impact do you envision your research having on the broader scientific community or various industries?

NV: So what we are still learning is that people, I have been getting contact by people that ask me about how you think, can you help us how this dye degradates? Or can you tell us what's happening to the dye? Can you see if, you know, with the dye library, can we find a dye that is better? Or, you know, we are doing some work with University of California, San Francisco, that they use this technology, differential scanning fluorometry. So they are doing a study for, unfolding of proteins to understand degenerative diseases, and they use a dye on it. And we have a collaboration, we have a grant with them, and you can see how our work has gone to a different area, and the dye library is using in that sense. So, we start seeing more impact on, you know, not only the level in the U.S., we have seen some collaborators in Europe, too, at this time. So it's nice to see some from time to time, someone contact me that I'm not aware. They say, hey, I have read your papers and can you help us on this area? So that's how I think our work has impact right now the community and especially in the dye field. Most of the work that has been done in dyes under my tenure here in NC State has opened a lot of doors for me and keep opening at this time.

LD: So it is a really vast field that mass spectrometry is used. So how do you keep up with the latest developments?

NV: Well, you know, I try to keep reading the latest literature. We have a great group of vendors. I'm part of right now what we call the Triangle Mass Spec Group here in North Carolina. I'm one on the board, the directors there, I'm the treasurer at this time. So we always invite the people that are in the top run of mass spectrometry. That's one way. The other is, you know, keep up with what people are doing. And you can see it's like sometimes like fiction, it's like, you expect this will not happen and it's happening now. So, you know, we try to always be in the forefront and see what are the new instruments, what are new advances. And one of the things we have in NC State, which is nice too, is this center called Metric, which is a great facility for us that has top-of-the-line mass spectrometers, NMR, and x-ray. So if I need something specific or more high-end instrument or mass spectrometer that they can provide and help, you know, I can easily access and learn from that or I would say, or NMR, so confirmed SIG. So I think in that sense, we try to be in the forefront. I think now ion mobility is a big mover on the field because help us separate before the mass spec, even things that were not very easy to do in HPLC. So I think that's how we try to, I try to keep up and try to see who is doing what. It's still hard because now it's popping up so much information that... But we do our best.

LD: So if somebody would be interested in pursuing a career in mass spectrometry or in dye characterization, what advice would you give them?

NV: You know, learning that mass spec is so broad, and I can tell you this because we have our annual here, the biggest mass spec conference is from the American Society of Mass Spectrometry, normally it's in June. This year, because I'm going to Finland, I will be missing that conference in Anaheim, California. But it's something that, for example, for my students is we have easily 600 persons per day from different fields. You can see, imagine for four days how many posters you can see, plus so many oral sessions, that is a high impact to see how much people are working. So you go to one of these conferences, you can see that everybody that is around you works in mass spectrometry somehow. So it's a great field. And the thing is, if you learn about mass spectrometry, not only you can be in the dye field, you can go to the proteomics, metabolomics, you know, medicine. So it's very broad. So mass spectrometry knowledge can send to different fields and can be very useful to a lot of researchers, not only chemists, but it can go to medicine. We have good friends that are doing great advances in medicine, especially for cancer research. So it's a big feeling for life for me is it's a way to learn more about the, you know, how we can help make things easier for the people.

LD: Thank you. My last question is that when you think about the Biocolors2024 conference and you close your eyes, what color do you see?

NV 1: Oh, I always like blue. One of my favorite colors. So it's nice. It's one of the colors that have been on my attention for a long time. Yeah, but it's just what I see. It's great to see and be part of Biocolors. So it's awesome.

LD: Okay, so I'm hoping that you see the blue also here in June with our blue skies and blue lakes and the blue in our Finnish flag.

NV: Yes.

LD: So thank you, Nelson, so much for this interview. It was very inspiring and informative.