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## Omics Informatics is providing Bioinformatics, Next Generation Sequencing Data Analysis, and H/D Exchange Software Solutions to propel Drug Discovery Research

Bruce Pascal  
President

Omics Informatics LLC

Contact:  
CEOCFO Magazine  
570-851-1745

**"This is the most highly cited software in the field." - Bruce Pascal**

Interview conducted by:  
Lynn Fosse, Senior Editor  
CEOCFO Magazine

**CEOCFO: Mr. Pascal, what is the concept behind Omics Informatics, LLC?**

**Mr. Pascal:** My company handles a number of different services. We do all kinds of Bioinformatics. We do next generation sequencing data analysis all the way to software development and custom software solutions. One of the main products we will talk about today is called HDX Workbench, which is a data analysis desk top platform, for the analysis of hydrogen exchange mass spectrometry data.

**CEOCFO: What are the challenges in looking at that data? What comprises the data and why is it difficult to work with?**

**Mr. Pascal:** Essentially, the interrogation of proteins is where it is at, because proteins relate to function in our biological system. Hydrogen exchange, coupled with mass spectrometry, is kind of a cost effective way to analyze the kinetics between protein-protein interactions, protein-ligand interactions, epitope mapping experiments and more. At a very high level, it basically involves taking a protein and incubating in deuterium or heavy water, for a certain amount of time at various time points. Then you have an enzyme like pepsin, digest it and then it goes into the mass spectrometer where everything is measured. Then you plot the rate of exchange difference, how fast the H<sub>2</sub>O turns to heavy water for each particular peptide, which is a protein fragment, the rate of exchange.

You could measure that in multiple different conditions, such as free and ligand bound or control and antibody conditions and then you could gain information as to where the binding site is, for example, in that type of experiment. Why is it difficult? Historically, it involved an enormous amount of data analysis. For example, in a typical HDX experiment you might have seven time points, times three replicates in two sample states. Therefore, you are looking at forty-two spectra for each protein fragment. You might have five hundred peptides or protein fragments, so it's over twenty thousand spectra that you have to actually go through and make sure that you are calculating the max of each. It has historically been very difficult. In about 2007 I published a paper called, The Deuterator, and we later published HD Desktop and now this is the third version of the software that we have developed as HDX Workbench. This is the most highly cited software in the field.

**CEOCFO: Would you tell us about HDX Workbench?**

**Mr. Pascal:** HDX Workbench was designed to manage and speed up the process and visualize and help researchers understand the hydrogen exchange from the mass spec data. What it does is it allows the users to just put in all their raw files and it automatically detects all of the peptides where they are in the mass spectrometry data and presents the results in a visualized interface. It does all of the searching automatically, allows everything to be presented and allows users to

correct things if necessary, exactly in the way that they were trained as mass spectrometrists, so they can change the retention time and they or mass range of each peptide replicate. Therefore, once that is done and we have masses for each isotopic envelope, then we have all kinds of visualization tools that can, for example, plot it on to a sequence covered heat map. We can automatically render things onto a 3D protein structure, which makes it much easier for people to understand and present what is going on.

**CEOCFO: *What were the challenges in creating the solution? What was harder than you thought it might be and what might have been easier?***

**Mr. Pascal:** It was a lot of data to go through, so we had to come up with new solutions. A very big challenge is to algorithmically detect the peptides very accurately. The more accurate it is, the less people have to change the results later. We had to invent and develop new ways to visualize the data and organize and manage it as well. Those are the difficulties.

**CEOCFO: *Is this available today? Is it still in development? Where are you?***

**Mr. Pascal:** It is a commercially available solution at [hdxworkbench.com](http://hdxworkbench.com). We do have an academic discount. Historically, it was made freely available for a number of years to the Scripps Research Institute where it was developed. However, now because I am a commercial entity and we need to continue supporting it we do charge for the updated version. It is available today and we are constantly evolving the product.

**CEOCFO: *Are people ready for it? Are they looking for something better?***

**Mr. Pascal:** There is a healthy demand, so the field of HDX has been growing tremendously. We regularly plot the number of publications and it just looks like an exponential curve. People are going all in on this technology, because it is cost effective and now there are automation and data analysis solutions. People are definitely ready for this. There is a huge demand for this to be even faster and more accurate. Therefore, it is ready today. People need it and people want it to be improved tremendously as soon as possible.

**CEOCFO: *What is your business model?***

**Mr. Pascal:** My pricing structure is subscription based. I charge, what I consider, to be a reasonable price and then I have other types of discounts for legacy customers and then higher support customers. However, what I am basically looking for are regular customers and recurring revenue, year after year. Therefore, they purchase a subscription to the software and with that they get the software, all of the updates, they can install it within a particular lab and get all of the updates and support from our team for one year and then every year they just renew it.

**CEOCFO: *How have you made it easy to understand for the user or does it matter if it is easy if it does what you need it to do?***

**Mr. Pascal:** This is a high specialized solution, so we would expect the users to have a solid understanding of what and HDX experiment is. Usually, they are mass spectrometrists and we do have a series of tutorials to help people through the software. We produce a lot of visualization tools to it to make it very easy to understand what the results are and we are always available to provide support and or demonstrations. A core philosophy that we had in designing the product is that every time you synopsized data you allow the user to go back one step and see what was involved in making up the synopsized data.

There is about five different levels of synopsizing data and we let the users see whatever level they want. For example, we could just produce the final result, which can be a 3D protein structure, overlaid with all kinds of fancy colors in the heat map and tell them that the blue section is probably the binding site, but when they want to understand what went into that then they could see the individual residues and then they could see the consolidated sequence coverage map and the individual peptides and then all the way back to the spectrum. We make it very transparent, but yet easy to understand the process.

**CEOCFO: *How often would someone use it? Daily, weekly or monthly? Is it part of standard working procedure? How do people interact day to day that have this system?***

**Mr. Pascal:** In a typical lab a pretty healthy HDX experiment involving two sample states could be acquired in a mass spectrometer if you have a robotic system in a period of six hours. Every six hours that mass spec can produce a new data set that needs to be analyzed with the software. Therefore, in a very efficient laboratory you could need to run the software twice daily. Usually, it is a lot less frequent than that, but that is about how often they would need to use it.

**CEOCFO: *Are there similar products available or have people been trying for something that will do what you can do? Are you ahead of the game?***

**Mr. Pascal:** There is always innovation in this area and I think it is great. However, going back to about 2002 there have been all kinds of different products and publications in this area. Those are two commercially competing solutions, but there is a whole slew of publicly available academic software solutions. In addition, publications are always coming out with new solutions, approaches and algorithms to solve problems in the field.

There are about twelve different solutions that have been made available. The problem when they are developed in an academic setting is one of continued support. This means if you do not continually support a software solution it will eventually expire, because something needs to be fixed when there is not funding to do that or expertise. Therefore, when you have a commercially backed product then you have the means to support it and keep it cutting edge.

**CEOCFO: *When you present your solution to people in the industry do they readily understand? Do they jump on board? What do you find when people learn about HDX Workbench?***

**Mr. Pascal:** I find that most of the customers know exactly what they want to see from HDX data. They know where they want to go. They know what their data looks like. They just want you to show them that they can get there. I think when you show them the final visualizations they immediately understand that the bigger solution could provide what they need.

**CEOCFO: *When you attend a conference, how do you stand out? There are so many ideas at one time in one place. How do you gain the attention you deserve?***

**Mr. Pascal:** In this particular market it is a very small field. Everyone knows everyone. In this case marketing means a little less and innovation means much more. I think if you are constantly updating your product with the latest and greatest features, then you could definitely make an impact in the field. Therefore, this June at the ASMS conference I am going to be presenting for example the capability of analyzing ETD data, which produces fragmentation mass spectrometry data that allows you to determine the rate of exchange at the residue level. That is one thing that many people want and will want more of in the near future.

**CEOCFO: *What is ahead for Omics Informatics? What should we expect a year from now?***

**Mr. Pascal:** We are constantly trying to forge new partnerships. We are trying to develop new software solutions. We are just rolling out a new service to next generation sequencing data analysis on a per sample basis. Therefore, we are basically expanding our product line and services. We intend to push in all of these directions and hope it leads us to the road to success.