

The CVUA Karlsruhe saves months of work using LOGS to organize and prepare spectroscopic data



Baden-Württemberg
Die Untersuchungsämter für
Lebensmittelüberwachung
und Tiergesundheit

Challenge

The CVUA¹ in Karlsruhe spent months on getting their data prepared for their analysis. The data was sorted manually according to specific criteria in a very time-consuming process. With rising number of criteria, the time needed to sort the data increased exponentially. Trying to find the required NMR spectra using the related metadata was a challenging process.

Solution

Today, the CVUA scientists sort data with a couple of mouse clicks, using LOGS² features. LOGS automatically uploads all data from the spectrometer and through search and filter functions makes it permanently accessible for further investigations, linked with all relevant metadata.

The Chemical and Veterinary Investigation Office (CVUA) in Karlsruhe is part of the governmental food and feed control for the federal state of Baden-Wuerttemberg in Germany. It is responsible for consumer protection – especially in regard to sanitation and deception – and the prevention of animal illnesses. Thus, a wide range of products, from food to cosmetics and pharmaceuticals to animal feed, are investigated using various analytical

methods including Nuclear Magnetic Resonance (NMR) spectroscopy.

Using three NMR spectrometers, the CVUA Karlsruhe examines around 6,000 samples every year, 1,100 of which are beer samples. The beer division is part of the beverage department, which is also responsible for drinking water, non-alcoholic beverages and liquor. For their chemometric analyses, the CVUA relies on sample metadata and NMR ex-

periments that are investigated statistically using principal component analysis (PCA) combined with linear discriminant analysis (LDA).

Organizing data for analyses is challenging when metadata and spectra are not linked

For combined PCA-LDAs, experimental data is sorted according to specific metadata criteria. In the case of beer,

¹ Chemical and Veterinary Investigation Office – <http://www.ua-bw.de/pub/default.asp?subid=2>

² LOGS data repository – <https://logs-repository.com>

this includes: type, origin, year, type of fermentation and more. “The major challenge for our investigations was

“We were missing the connection between the metadata and spectra – a huge problem.”

Dr. Tobias Brunner, project leader at the CVUA

the very time-consuming manual sorting of the data by different criteria,” said Dr. Thomas Kuballa, head of the beverage and NMR spectroscopy department since 2012. “In the case of beer, our chemical lab assistant took about two months in addition to his regular work to sort the data by selected criteria in a spreadsheet. This is very dull work.”

The larger the number of criteria, the longer it takes to establish the spreadsheet, which is used to find the required spectra that are needed for the PCA. “This approach was not practical for the analysis due to time and labor,” said Dr. Tobias Brunner, project leader at the CVUA. “It was a tedious job. A co-worker was busy creating and maintaining the spreadsheet, while I was going through the folders looking for the spectra and copying them. [...] Any time we were looking at a slightly different approach we had to change the criteria and start all over again.”

The team at the NMR department had established a well-organized data turnaround for their analyses before. They

were already using a laboratory information management system (LIMS) and their own sophisticated system for data storage. The data was copied into a complex, structured subfolder system. “The data was saved in a folder labeled with the measurement date, but was missing other metadata,” said Thomas, who played a key role in establishing ^1H NMR spectroscopy as an acknowledged method at the CVUA in Karlsruhe. Tobias recalled: “We were missing the connection between the metadata and spectra – a huge problem.

The spreadsheet with the metadata was stored at one location, and the spectra were stored elsewhere.”

These challenges caused Thomas to look for a general solution to deal with the metadata sorting process. He wanted to create a system that was clearly defined and less time consuming. The first time he was introduced to LOGS, he thought: “This is exactly what we need for organizing our data.”

After first trials, his team wished for additional specific functionalities in LOGS and communicated their needs to the SIGNALS³ developers. “I was surprised how flexible and open the people at SIGNALS were to our needs. This is not something that happens very often in business. I was very happy about that.” He also felt that working with SIGNALS was very easy and pleasant: “As scientists, they speak the same language, which makes communication much easier.”

Using the filter and search functions data can be sorted by any criteria, saving months of work

After only three months, SIGNALS developers had implemented the custom features and LOGS had become part of the lab routine at the CVUA Karlsruhe. “This was rather fast for software that had to be adapted to our needs and had to be implemented into our workflow,” said Thomas. The CVUA is now able to filter and sort their NMR data according to any criteria. From there on the data is exported to a file, which is used as input for the PCA. “When I first saw the sorting of NMR data using the LOGS filter feature, I was impressed. It only required a couple of mouse clicks to get the data ready for the analysis. This used to take months of work,” said Thomas. “I was positively surprised that LOGS worked from the start. I have been working with large equipment and its software in the organic and inorganic department for 25 years and this is not always the case.”

“When I first saw the sorting of NMR data using LOGS, I was impressed. This used to take months of work,”

Dr. Thomas Kuballa, head of the beverage and NMR spectroscopy department

Spectra and relevant metadata are parsed and uploaded automatically

“When I learned about LOGS, I was very happy because it sounded like it would

³ <http://logs-repository.com>

save us a ton of work”, said Tobias, who earned his PhD in a synthesis lab in Karlsruhe prior to working for the CVUA. Instead of implementing the metadata right before the PCA is performed, it is now included into their already established LIMS from the start. “We’ve always entered metadata partially anyways, so now we import all of it,” said Tobias.

The metadata is imported from LIMS into BRUKER SampleTrack™, which connects the data and the NMR experiment. LOGS automatically uploads all measured data from the spectrometers as soon as the experiment has finished, and additionally reads and imports the relevant metadata for each dataset. Now, in LOGS, the data may be sorted by any criteria using the filter and search functionality, after which it is exported to a file for PCA.

The CVUA team had to agree on useful tags for their analyses: “You have to create and enforce the tagging conventions, but compared to the previous manual sorting process, it’s nothing,” said Thomas. “Everybody on the team thought that LOGS was great. They saw the many options the system was offering for our analyses in the future.”

“We can perform a lot more analyses now and with LOGS our options increased exponentially. I can create as many spreadsheets as I want per day with LOGS to answer different questions.”

Dr. Thomas Kuballa, head of the beverage and NMR spectroscopy department

A lot more analyses can be performed now paving the way for an increasing amount of samples in the future

Extrapolating the amount of samples over the next ten years, the CVUA is expecting to compare more than 10,000 beer samples alone, so the time savings through LOGS will only increase over the coming years. The more data is used in the PCA, the better its outcome. “LOGS made the analysis of our data easy and fast,” said Thomas. “We can perform a lot more analyses now and with LOGS our options increased exponentially for the coming years.” This is also acknowledged by the rest of the team at the CVUA. “If I want to, I can create as many spreadsheets as I want per day with LOGS using different

criteria in order to answer different questions,” said Tobias, who also liked working with the SIGNALS team. “They know the challenges and hurdles dealing with a torrent of spectra. [...] The collaboration with SIGNALS is great, especially regarding the support. Someone is always available and I always get an answer.”

In the future, Thomas and his team see many opportunities for their analyses using LOGS: “SIGNALS lived up to their promises.” The CVUA team has already requested an API from SIGNALS, which will automate another step in their analysis process. Other CVUA departments have already registered their interest in LOGS as well.

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