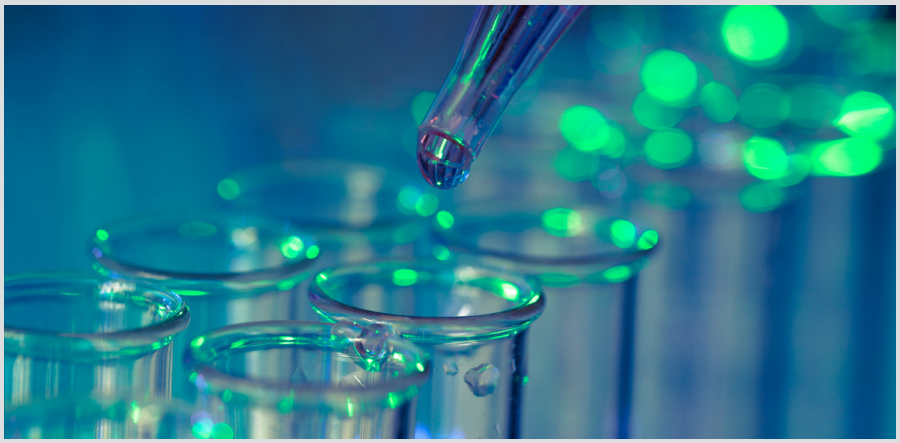
ALICE2 Case Study

Mylims: An outstanding experience for open, free-of-charge and online data management and manipulation of Nuclear Magnetic Resonance spectres.

Through the advanced networks of Latin America (RedCLARA) and Europe (GÉANT), a group of researchers developed an application open to the entire scientific community. Five years after its beginning, the initiative has been applied with impressive results in areas like coffee and medicine; it has regular users, is used in the field of education and has been the starting point for other projects.

"This platform makes it possible to share data, but not only data, also the analysis of these data. To do this it is necessary to be able to extract, in the most efficient way, the information obtain with NMR (Nuclear Magnetic Resonance) experiments. This information makes it possible to understand at an atomic scale the composition of a sample. This way, we enable equipment worth more than a thousand million pesos work continuously and not only during regular working hours", explains the chemist and researcher Julien Wist, who created and implemented Mylims (My Laboratory Information Management System), with the support of Luc Patiny from Switzerland and Edgar Daza and Cristian Blanco from Colombia.

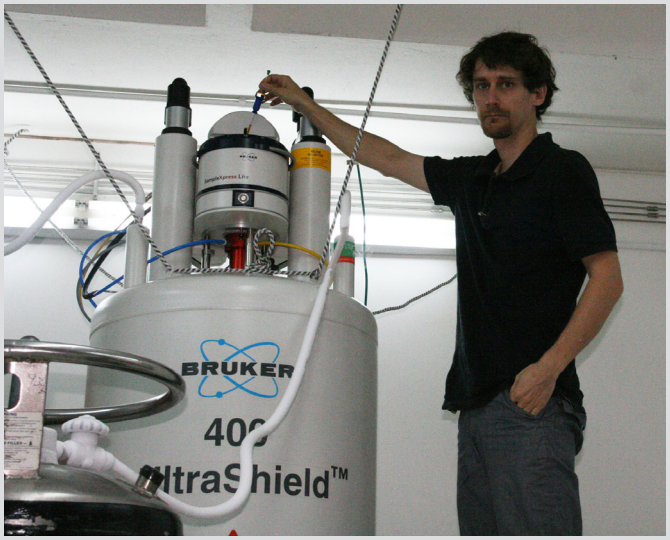
The initiative makes available for the scientific community a powerful tool which makes it possible to freely, openly and from any computer connected to the internet, process data, manipulate spectres, interpret results and then compare them with the spectres obtained by other users and which are stored in databases.



The Mylims applications comprise work in the field of chemistry and medicine. This way, according to Wist, having access to this kind of information enables, for instance, the identification of the compounds present in a mixture, the comparison of two mixtures or the diagnosing of illnesses. *"Our group has managed to build an expert system to detect frauds in coffee and has detected several real cases for the local industry (Almacafé). It also makes it possible to compare extracts from healthy cells and extracts from leukemic cells (collaboration with the group of Ismael Samudio, Javeriana Bogotá), and we hope it enables us to find out which compounds, biomarkers, are responsible or make the illness evident. Furthermore, there are already antenatal NMR diagnoses and there are several examinations which detect illnesses through urine by making use of NMR to identify abnormalities, thanks to the pioneering work of a group of scientists from Imperial College London"*, he adds.

What are the results of this experience?

Wist states that: *"There are around two hundred users who work every day with our system. There are developers who want to get on board and use our tool to unify the analysis of spectroscopic data. There are virtual courses based on our tool and using our data. Three companies fund our effort. We have a project with funding from Europe, which involves six groups from six countries to further develop the subject of solid-state NMR. Our tools get more than two thousand daily clicks; we are first in Google (nmrbd.org is where the lims' tools are described) competing with very well known programmes; our article on the simulation of spectres was the most downloaded on the Journal of Magnetic Resonance during two months; the poster by my student Andrés Mauricio Castillo received an award last year... and we still like what we do!*



Network in use

For the project's development the team used the connection of Colombia's national network, RENATA, with RedCLARA: *"This procedure would be pointless without a fast network. We are talking about resonance spectres which can be up to 128 Mb and the idea is to work with them in a network, that is, they have to be uploaded and downloaded in ideally less than two seconds and that would not be possible without an ultra high-speed network", indicates Julien Wist and he adds "we want to take advantage of grid computing to be able to predict a certain amount of properties for each molecule; this also requires a good connectivity".*

mylims.org

The site features a guided tour, information on how to use it (applicable to e-learning environments) and a section for frequently asked questions that includes information on the platform's functioning, system requirements and exercises.

More information:

http://www.mylims.org
http://www.nmrlab.org/

RENATA: http://www.renata.edu.co/index.php/component/content/article/5-noticias/2525-colombia-tiene-una-de-las-mas-altas-cobertura-en-banda-ancha-de-america-latina-hecho-que-tenemos-que-aprovechar-para-educar-y-hacer-ciencia.html

This Project is funded by the European Union

A project implemented by RedCLARA

It is very important to have a high-speed data transmission network which enables the connection between the different actors in the process of sample analysis using NMR in Colombia. A dedicated network makes it possible to upload the files to the mylims server and make the analysis quickly. It also enables fast access to the database, so that results can be matched against those obtained by previous users.

Cristian Blanco Tirado, *Professor at the School of Chemistry and Vice-Chancellor of the Universidad Industrial de Santander (Colombia)*

Nós estamos desenvolvendo a ciência para reduzir a diferença entre países em desenvolvimento e desenvolvidos, e uma rede de Internet eficiente realmente ajuda. A capacidade de cálculos em grades computacionais oferecida pela GÉANT-RedCLARA foi importante para desenvolver o projeto. Hoje não há mais opção que oferecer excelente conexão, não somente para a pesquisa, mas também para a formação de estudantes.

Luc Patiny, PhD, Director of Chemical Information
Federal Polytechnic School of Lausanne (EPFL), Switzerland