



SOCIÉTÉ CHIMIQUE DE GENÈVE

New challenges in the management of chemical information

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A lot of chemical information is generated everyday in the laboratories. They include reactions, chemicals, physical characteristics, spectra, biological results, images, ...

While a lot of attention has been focussed on the storing of all the data and the possibility to retrieve it easily, we should not forget that the final goal is to extract some knowledge from this information. A typical example concerns the high-throughput screening results for which a lot of attention has been devoted. This is not however the case for spectra for which available tools are still surprisingly limited when dealing with leading research.

During this talk we will show the different aspect about saving, retrieving, processing and extracting knowledge based on some real case examples in the field of nuclear magnetic resonance spectroscopy and mass spectrometry. Most of the examples are based on open source projects and allow to efficiently manage all the chemical information directly from a web browser.

Conférence présentée le

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Auditoire A. Pictet – A100

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La conférence est publique

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