Visualization and processing of chemical information in the browser

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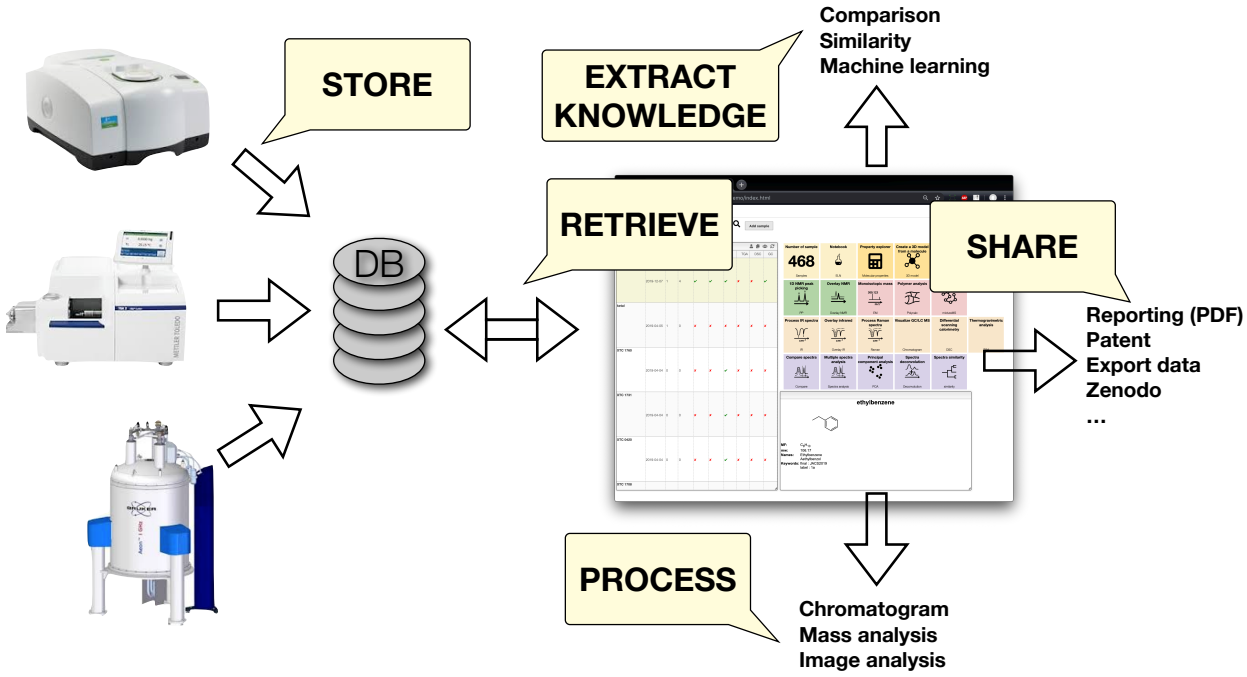
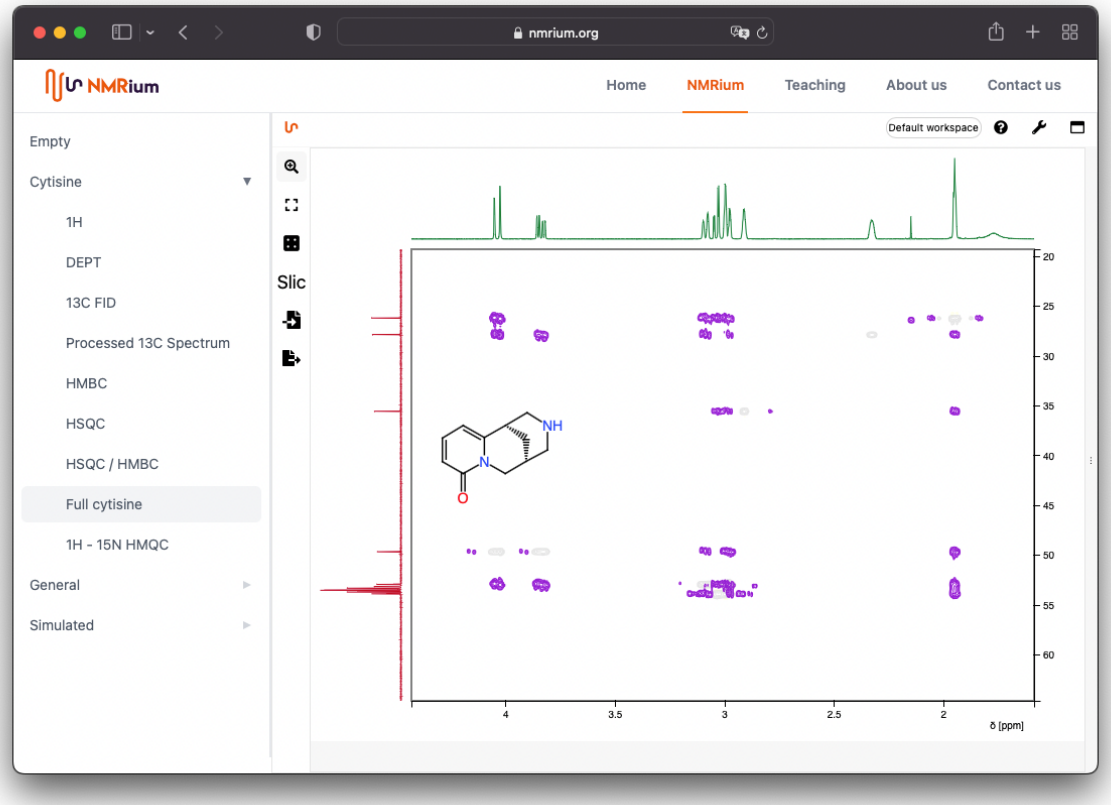
Nowadays, computers come with a browser pre-installed, and many web applications have been developed to perform everyday tasks such as webmail, maps, document editing, etc. The main advantage is that no software needs to be installed and updating is done by simply reloading the web page. Moreover, this approach is cross-platform and the data can be accessed from anywhere.

For over 20 years we have been dealing with data workflow and the idea of storing data in a database as quickly as possible and processing it directly in the browser. This is done with the help of over 150 JavaScript libraries that have been developed over the years.



Analytical data workflow

In this presentation, we will show how data can be stored, retrieved, processed, and eventually knowledge can be extracted from it [1], using **www.c6h6.org** as an example [2]. We will present an advanced application of mass spectra analysis of polymers (**www.polycalc.org**) performed directly in the browser [3]. Finally, we will present **www.NMRium.org**, a freely accessible website that allows to visualize, compare and process NMR spectra [4].



Example of browser web application for NMR data processing

[1] Jablonka, K. M., Patiny, L., & Smit, B. (2022). Making the collective knowledge of chemistry open and machine actionable. *Nature Chemistry*, *14*(4), 365–376.

[2] Patiny, L., Zasso, M., Kostro, D., Bernal, A., Castillo, A. M. M., Bolaños, A., Asencio, M. A. A., Pellet, N., Todd, M., Schloerer, N., Kuhn, S., Holmes, E., Javor, S., & Wist, J. (2018). The C6H6 NMR repository: An integral solution to control the flow of your data from the magnet to the public. *Magnetic Resonance in Chemistry*, *56*(6), 520–528. https://doi.org/10.1002/mrc.4669

[3] Desport, J. S., Frache, G., & Patiny, L. (2019). MSPolyCalc: a web-based App for polymer mass spectrometry data interpretation. The case study of a pharmaceutical excipient. *Rapid Communications in Mass Spectrometry*. **https://doi.org/10.1002/rcm.8652**

[4] Patiny, L., Musallam, H., Zasso, M., Bolaños, A., Kostro, D., Wenk, M., Ahkrin, S., Jeannerat, D., Ziegler, E., Liermann, J., Schloerer, N., & Wist, J.. (2022). NMRium: ReactJS component to display and process NMR spectra (v0.33.0). Zenodo. https://doi.org/10.5281/zenodo.7258284