Resurrecting NMR spectra

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The prediction of NMR chemical shifts as well as the automatic assignment of spectra requires the knowledge of a large set of analyzed data. Only few databases of 1H NMR chemical shifts are currently available over the internet. The most exhaustive is probably the Japanese Spectral Database System that contains over 12000 1H NMR spectra. This lack of available data is probably due to the time consuming step of collecting and assigning the spectra to a searchable format.

In this poster we will present a new java applet that enables to assign a chemical structure to the NMR spectrum by drawing a line between an atom and an automatically characterized signal. Moreover this applet is able to recreate an NMR spectrum from published in-line experimental part. As an example we will show a database containing over 4000 resurrected spectra.