Quantitative NMR methods and automatic analysis of NMR spectra

Valtteri Mäkelä

NMR spectroscopy is widely used technique in chemistry, especially in organic chemistry. Usually it is used for structure determination and verification of pure compounds, but as instruments and methods have improved, also increasingly for qualitative and quantitative analysis of mixtures. The mixtures can be relatively simple, as in quality control of reaction mixtures or industrial processes, or very complex, as when analyzing biological samples with hundreds of distinct metabolic products.

Aim of my research is to develop better quantitative NMR methods, and tools for more automated analysis of quantitative NMR spectra. More specifically:

1. **Improving sensitivity and reducing signal overlap:** compared to many other spectroscopic methods, NMR has relatively poor sensitivity. The most sensitive commonly used isotope, ^{1}H, can deal with microgram amounts of compounds, but when analyzing complex molecules and mixtures it has a tendency to suffer from signal overlap, as the chemical shift dispersion is limited and coupling complicates the signal structure. ^{13}C NMR offers much improved resolution, but has natural abundance of only 1% rendering the sensitivity quite poor. The aim is to find improved techniques which reduce these fundamental problems of NMR.

2. **Spectral analysis and automation:** When analyzing mixtures, there are usually many signals and samples involved. There are few tools which are meant for analysis of this kind of NMR data, and many of those are commercial and/or vendor dependent. The aim is to develop new tools and methods for automated analysis of large numbers of quantitative NMR spectra.

Some of the produced tools are available at: http://vltr.fi/imatranmr/