EFFICIENT DECONVOLUTION OF COMPLEX MIXTURES BY COVARIANCE NMR

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Introduction

Analysis of complex mixtures plays an important role in many areas of chemistry and the life sciences. A new analytical method is described which deconvolutes the NMR spectrum of a mixture into individual components and spin systems. The method, which does not require hyphenation, is based on the analysis of covariance total correlation spectroscopy (covariance TOCSY) spectra of a mixture. Traces with minimal spectral overlap with other spin systems are identified, rank ordered, clustered, and compared with a NMR spectral database. The method achieves very good performance for several applications, which includes amino-acid mixtures and a decapeptide.

Results and Discussion

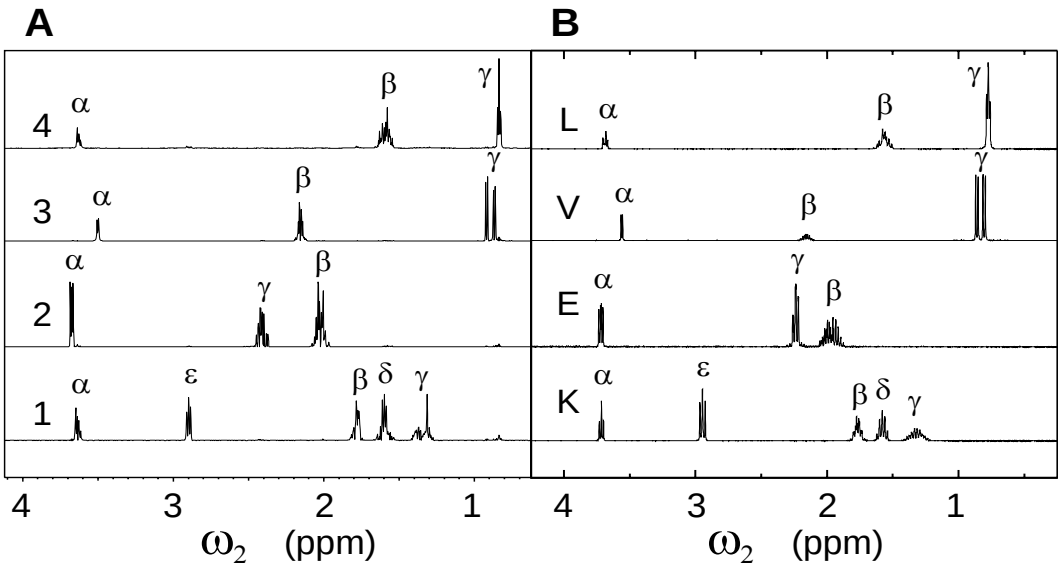

Figure 1 Results of the deconvolution method for a four amino acid mixture containing Leucine, Valine, Glutamic acid, and Lysine (Panel A) in comparison with 1D NMR spectra of the individual amino acids taken from the BMRB data bank.

The deconvolution method introduced in this work takes advantage of the high spectral resolution of covariance TOCSY spectra. The trace analysis based on the importance index and subsequent clustering is highly efficient providing realistic 1D spectra of the underlying spin systems. As NMR spectral databases, such as the BMRB metabolomics database, are rapidly growing, traces identified in covariance TOCSY spectra to represent 1D spectra can be (semi-)automatically screened against database entries to identify and quantify the TOCSY traces offering an efficient and reliable avenue for the deconvolution of complex biological mixtures.

Acknowledgements

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