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Metabolite analysis of biological mixtures using adaptable-shape modeling of an online NMR spectral database

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Using adaptable-shape modeling of ^{1}H NMR spectra for hundreds of metabolites present in the NMR spectral database at BioMagResBank (BMRB), we have developed a probabilistic approach and online implementation to perform metabolite identification in complex biological mixtures. The general approach includes spectral deconvolution of each entry in a basis set of spectra to create a parametric shape model and a set of alternative mathematical representations for the model designed to maximally distinguish between any pair of basis set entries. We show that probabilistic methods can be employed to estimate the likelihood that a given set of input spectra of a complex mixture contain evidence for the presence of detectable levels of a given compound subject to allowed deviations in the canonical frequency and line width characteristics of that compound. Relevance of this methodology to metabolomics is demonstrated by comparing the profiling of relevant biological samples (*e.g.* liver cell extracts and blood serum) by these methods to the same profiling of derived liquid chromatographic (LC) fractions. Evidence is shown that the set of compounds identified in these complex biological mixtures is consistent with the easily-identifiable compounds present in the component fractions. The program that perform this analysis is available as an online application that allows the operator to load processed ^{1}H NMR spectra (Bruker, Varian, NMR Pipe data formats) from their local computer, perform a search against a subset of modeled compounds in the spectral library, and graphically display the results overlaid upon the input spectra. Ensemble shape models have already been created for over a hundred ^{1}H spectra in the BMRB and active work is obtained at expanding this library to eventually include all ^{1}H spectral entries. The approach is fully extensible to 2D NMR experiments and incorporation of 2D ^{1}H-^{13}C HSQC spectra into the shape library.

Biography

Roger Chylla is an associate scientist and director of software development at the National Magnetic Resonance Facility at Madison (www.nmrfam.wisc.edu). He has published numerous papers in the area of maximum likelihood reconstruction of NMR spectra both for biomolecular NMR and metabolomics. His current focus in collaboration with BioMagResBank (www.bmrb.wisc.edu) is to make an online database of metabolite NMR standards available to metabolomics researchers through development of open source software platform for metabolite identification and quantification. He received his Ph.D. in biophysics at the University of Illinois in 1990 and has complemented his academic career with experience in cofounding a successful medical software company and in executive management of software teams.