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NMR Manager – Metabolomics software for interpreting NMR spectra

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Short Abstract: Metabolomics software developed to analyze/store NMR spectra; with the capability to graphically display and compare experimental and database spectra. Harnessing automated peak detection algorithms and statistical methods to compare experimental NMR against statistically generated populations of NMR, and identifying significant peak variations between NMR for rapid metabolite profiling.

Long Abstract:
Introduction 1H-NMR (Proton Nuclear Magnetic Resonance) spectroscopy is one of a number of complimentary techniques used to investigate metabolite pools within complex matrices and through data integration an aid for correlating findings using complimentary methods. Chemical groups are located within an NMR spectrum, which is used to identify metabolic compounds, making NMR an increasingly used technique in metabolomics research. NMR Manager is both a searchable database for storing, retrieving and viewing metabolite NMR spectra and associated peak information, e.g. peak height and peak position and an analysis software package. The software is designed to aid comparison and interpretation of one-dimensional NMR spectra to identify metabolites in complex mixtures using novel statistical methods and automated peak detection and search algorithms. Toolkit The software has a built-in toolkit that has a number of features. Both automated and interactive tools for setting reference peak positions within NMR. There is a graphical viewer to allow the user to perform visual comparisons between experimental NMR, and database spectra. Built-in functions for automated spectral alignments - database entries versus experimental NMR. A search engine allows manual retrieval of database NMR via inputting peak ranges in ppm for comparison against experimental NMR. Automated peak detection and assignment algorithms coupled with an automated database search engine. There are a number of statistical methods built into the software to calculate the variability within populations of NMR, which can be viewed through graphically generated plots within the software. These statistical methods can be used to compare experimental NMR with a particular phenotype against the generated populations of NMR to identify novel peaks and therefore metabolites. Graphical User Interface A viewing pane displays experimental NMR and peaks identified from the automated peak detection algorithm, which can be searched against compounds stored in the database. Other features include tools to zoom in on a ROI (region of Interest) within spectra, both on a single spectrum and simultaneously on the same ROI in the experimental and database NMR spectrum. Slider bars can be utilized to magnify peak intensities to identify metabolites at low concentration and to manipulate peak detection sensitivity. We have developed data visualization tools within the user interface for comparing peak area clusters in different populations of experimental NMR Discussion The software is currently being employed to identify metabolites in complex matrices. Using the

automated peak detection algorithm and search tool on experimental NMR matched peaks can be compared to thousands of NMR stored with the database. Returned database entries can be aligned with the experimental spectrum through a matched database. Through the aid of a graphical view of spectra, comparisons of both the position and shapes of identified peaks can be used to match particular chemical components. Statistical methods and automated peak detection/assignment algorithms also give rapid analysis to compare NMR experimental samples against populations of NMR. Enabling the identification of significant peak variations between samples and a population, to identify novel metabolites. We have also developed novel data visualization techniques to aid rapid data analysis. In the near future we aim to add to the software other NMR methods e.g. 13C-NMR coupled with various 2D (two-dimensional) NMR analytical techniques develop further statistical, analytical and visualization tools to improve the rapid detection of metabolites in complex mixtures. NMR along with a number of complimentary techniques provides powerful tools in metabolomics and along with data integration techniques is proving to be invaluable in systems biology. NMR Manager is designed to aid rapid comparison and interpretation of NMR spectra. The storage of NMR spectra data, and the development of statistical methods, peak detection/assignment algorithms and data visualization methods will reduce the bottleneck in data interpretation for metabolomics. Reference Adrian Charlton*,1, Theo Allnutt2, Stephen Holmes1, James Chisholm1, Samantha Bean2, Noel Ellis2, Phil Mullineaux2 and Sarah Oehlschlager1 NMR profiling of transgenic peas Plant Biotechnology Journal Volume 2 Page 27 - January 2004 1Department for Environment, Food and Rural Affairs, Central Science Laboratory, Sand Hutton, York, YO41 1LZ, UK 2John Innes Centre, Colney, Norwich, NR4 7UH, UK