

Complex Mixture Analysis by NMR (COLMAR) Metabolomics Web Portal at NHMFL

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Introduction

Identification and quantification of different chemicals is a key aspect of the emerging field of Metabolomics, which aims at the elucidation of the chemical fingerprint of biological systems. Nuclear magnetic resonance (NMR) spectroscopy has a unique potential for this task as it (a) does not require potentially labor-intensive and costly physical separation of the mixture components prior to measurements and (b) can provide quantitative concentrations of the different metabolites. We have recently developed three interrelated Covariance-based NMR metabolomics web servers or web portals, termed COLMAR (for Complex Mixture Analysis by NMR) for identification of components in Metabolomics mixtures.

Results and Discussion

Figure 1 outlines the steps for COLMAR analysis, which includes: Metabolomics sample collection, data collection using high magnetic field spectrometers and high sensitivity cryoprobes, covariance NMR processing, data clustering, DemixC analysis, and database query. Table 1 shows the three parts of the COLMAR metabolomics web servers. Covariance NMR processing has been made available previously as downloadable software from our website (<http://spin.magnet.fsu.edu>). Now, users can conveniently perform covariance NMR through our Web Portal. In a next step, the DemixC part of the Web Portal accepts 2D NMR spectra as input, and returns traces of individual components of the mixture. In the last step, the web query part of the web portal screens the DemixC traces against NMR spectral databases. The three parts of the portal can be used together or separately, depending on the specific needs.

Conclusions

The COLMAR Metabolomics Web Portals aid the identification and quantification of chemical components of metabolomics mixtures without requiring physical separation of individual components. This web portal, which allows users easy uploading and downloading of NMR data, should significantly facilitate the analysis of a wide range of biological mixtures.

Acknowledgements

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References

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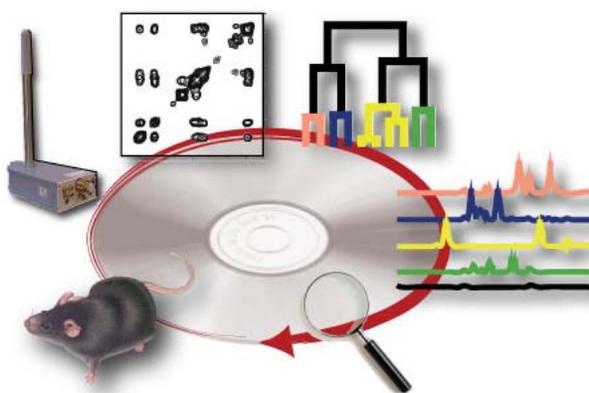


Figure 1. Complex Mixture Analysis by NMR (COLMAR)

Table 1 COLMAR Metabolomics Web Portal

COLMAR covariance

- <http://spinportal.magnet.fsu.edu/covariance/covariance.html>
- automatically generates a covariance NMR spectrum using Bruker, Varian, or NMRPipe data as input

COLMAR DemixC

- <http://spinportal.magnet.fsu.edu/demixC/demixC.html>
- identifies NMR traces of individual components of metabolomic mixtures

COLMAR query

- <http://spinportal.magnet.fsu.edu/webquery/webquery.html>
- automatically searches DemixC results against NMR databases