TOCCATA Metabolomics Database: A New Addition to the COLMAR Web Server

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Introduction

A customized metabolomics NMR database, TOCCATA, is introduced, which uses ^{13}C chemical shift information for the reliable identification of metabolites, their spin systems, and isomeric states. TOCCATA, whose information was derived from the BMRB and HMDB databases and the literature, currently contains 463 compounds and 801 spin systems, and it can be used through the publicly accessible web server http://spinportal.magnet.fsu.edu/toccata/webquery.html. TOCCATA allows the identification of metabolites in the submillimolar concentration range from ^{13}C−^{13}C total correlation spectroscopy experiments of complex mixtures, which is demonstrated for an Escherichia coli cell lysate, a carbohydrate mixture, and an amino acid mixture, all of which were uniformly ^{13}C-labeled.

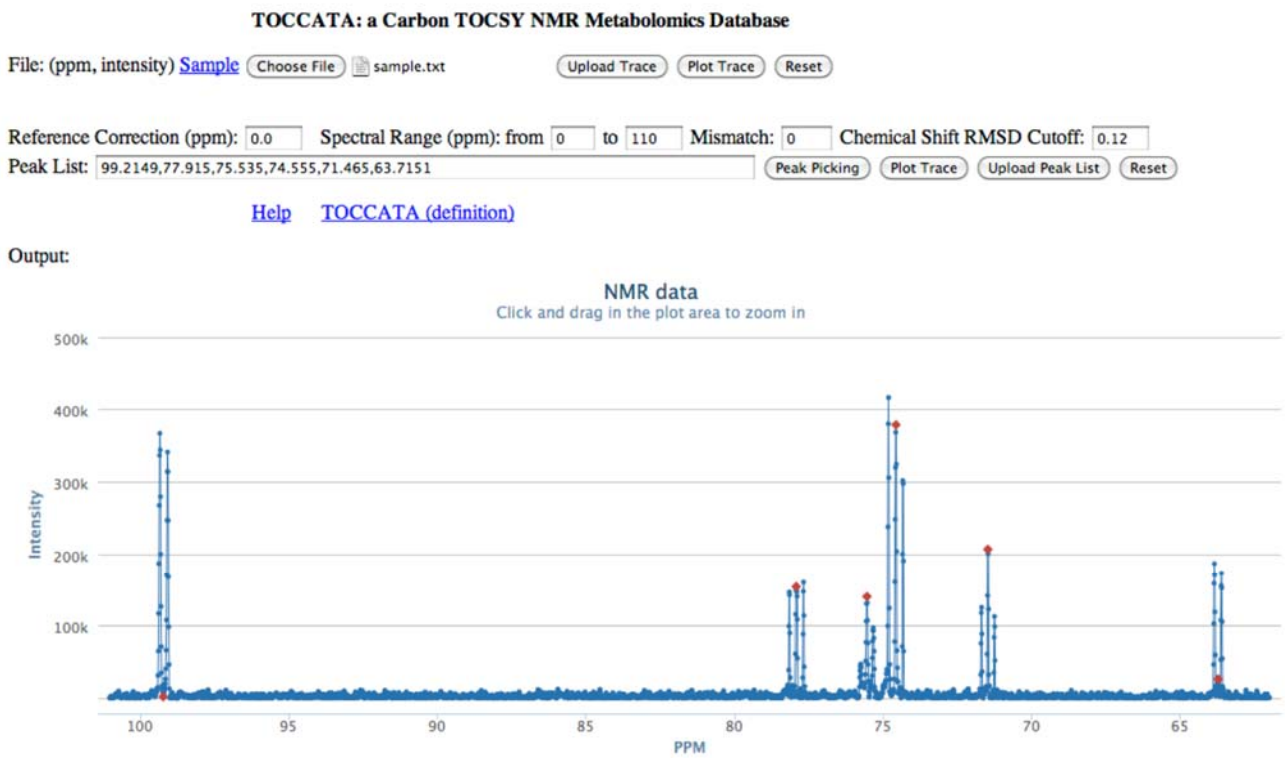

Figure 1. Screenshot of the TOCCATA web server user interface. A 1D ^{13}C TOCSY trace of interest can be uploaded and interactively peak-picked (red diamonds) with the corresponding chemical shifts displayed in the peak list. Querying of this peak list against the TOCCATA returns the best matching compound.

Conclusion

Unambiguous identification of the components of complex metabolite mixtures is a key step for their biological interpretation. The TOCCATA database produces ^{13}C TOCSY traces that yield database query results in a very high accuracy of compound identification for samples that are uniformly ^{13}C-labeled.

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