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Generalized Tree Structure to Annotate Untargeted Metabolomics and Stable Isotope Tracing Data

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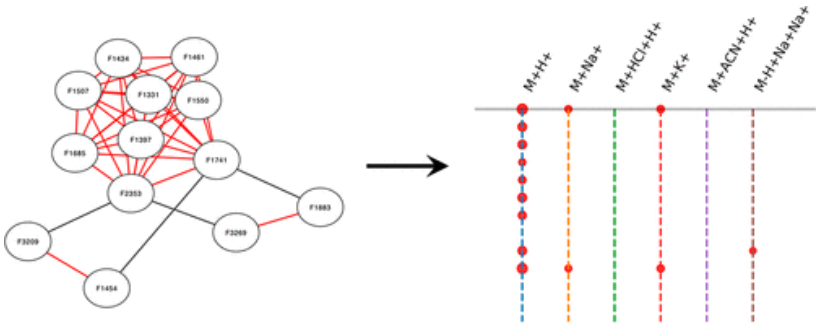
SUBJECTS: Adducts, Ions, Isotopes, Metabolomics, Software

Abstract



In untargeted metabolomics, multiple ions are often measured for each original metabolite, including isotopic forms and in-source modifications, such as adducts and fragments. Without prior knowledge of the chemical identity or formula, computational organization and interpretation of these ions is challenging, which is the deficit of previous software tools that perform the task using network algorithms. We propose here a generalized tree structure to annotate ions in relationships to the original compound and infer neutral mass. An algorithm is presented to convert mass distance networks to this tree structure with high fidelity. This method is useful for both regular untargeted metabolomics and stable isotope tracing experiments. It is implemented as a Python package (khipu) and provides a JSON format for easy data exchange and software interoperability. By generalized preannotation, khipu makes it feasible to connect metabolomics data with common data science tools and supports flexible experimental designs.

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Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.analchem.2c05810.

- User manual and Jupyter Notebook (PDF)

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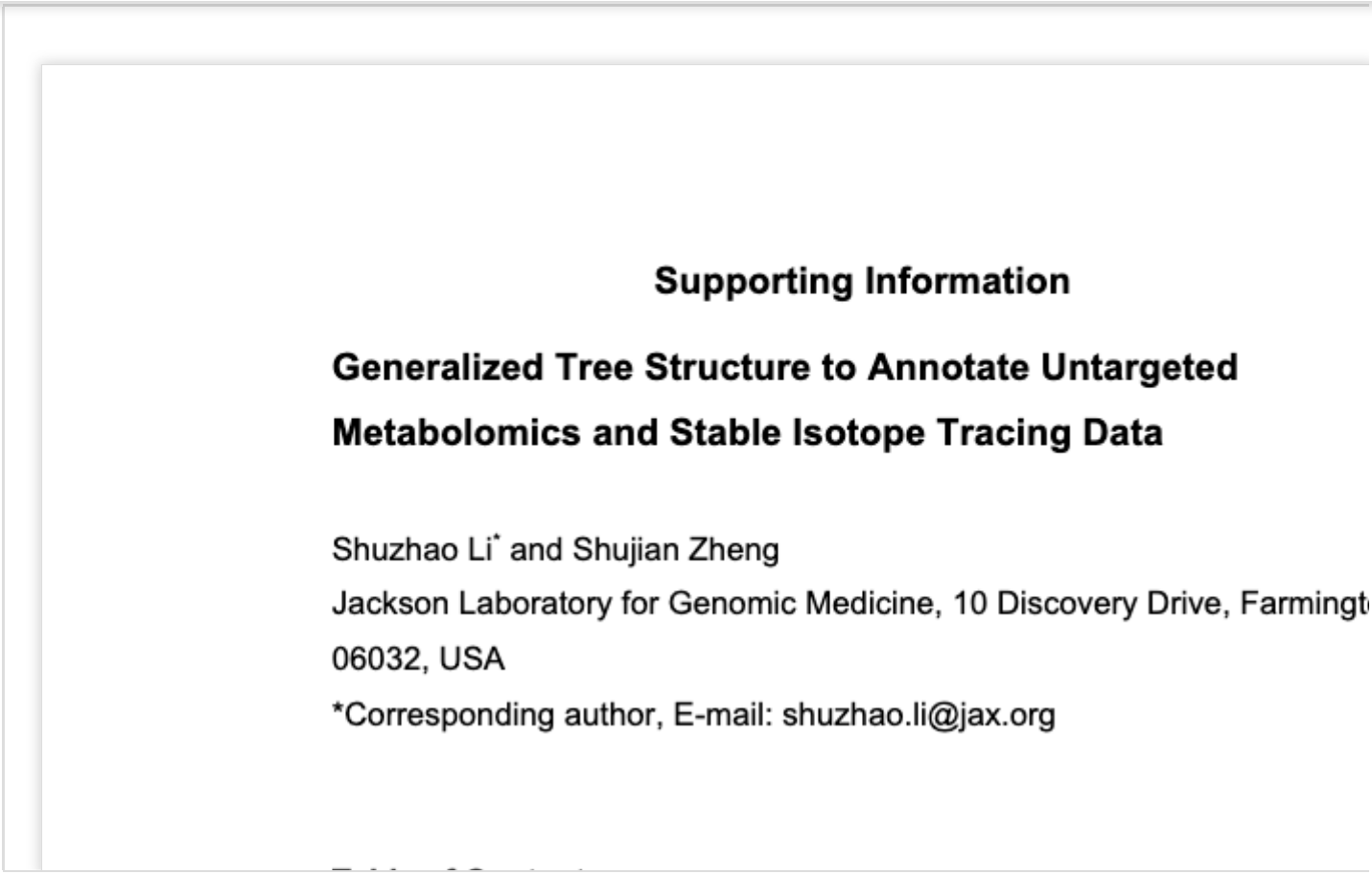

Supporting Information

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