Simulating Metabolism and $^{13}$C Isotopomers

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**Summary:** A MatLab-based program is presented for predicting $^{13}$C NMR spectra and mass $^{13}$C isotopomer data of various tissue metabolites in a $^{13}$C tracer experiments. The interface shown in Figure 1 allows the operator to select any $^{13}$C-labeling pattern for glycerol, lactate, fatty acids or CO$_2$ (for possible labeling via a carboxylation pathway) and to choose relative activities of PDH (pyruvate dehydrogenase), $\gamma$PC (pyruvate carboxylase), TPI (triose phosphate isomerase), GK (glycerol kinase), and PK (pyruvate kinase). The output provides calculated $^{13}$C NMR spectra for all 3-5 carbon TCA cycle intermediates, alanine and lactate, and glucose for those tissues undergoing active gluconeogenesis. The program is useful for predicting changes in $^{13}$C multiplet patterns in NMR spectra and changes in mass isotopomer ratios in mass spectral data as a tissue responds to changes in flux of various substrates through completing pathways involving mitochondrial metabolism. The program tcaSIM$_2$ (copies available free of charge) is also valuable for teaching metabolism and analysis of $^{13}$C NMR data and mass spec data in metabolic tracer experiments.

**Bio:** A. Dean Sherry, PhD, is Professor of Chemistry at the University of Texas at Dallas and Professor of Radiology at UT Southwestern Medical Center in Dallas. He holds the Cecil & Ida Green Distinguished Chair in Systems Biology at UT Dallas and serves as Director of the Advanced Imaging Research Center at UT Southwestern.

**Publications related to this topic:**