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# <sup>13</sup>C Metabolic Flux Ratio Analysis by ChemAdder - from 2D HSQC to virtual 1D spectra and qQMSA

NMR spectroscopy is an efficient method for obtaining quantitative data on the fractional 13C enrichment of metabolic intermediates or end-products. In biosynthetically directed fractional 13C labelling using uniformly 13C labelled carbon source, the biomass becomes 13C labelled in a metabolic flux distribution dependent manner and the cleavage and the formation of the covalent bonds of the carbon backbone differing between the alternative pathways is monitored from the 13C-13C scalar coupling fine structure of 13C NMR spectra. The 13C-13C couplings give rise to from two to four multiplets per carbon. These multilplet components are most conveniently observed and integrated from HSQC spectra. The integrations of these heavily overlapping signals, however, is very difficult using conventional NMR software.

In quantitative Quantum Mechanical Spectral Analysis (qQMSA) it is assumed that an NMR spectrum is a sum of the model spectra of its components and the experimental spectra are replaced by models obtained by fitting the spectra using Quantum Mechanical (QM) theory. This results in spectra pure from impurity signals, noise and other artefacts, but interpreting even the smallest spectral details.

We present a special software ChemAdder capable of 13C assisted fluxomics. The HSQC spectra of the cell hydrolysate are first converted to virtual 13C-13C coupled 1D 13C spectra of each amino acid. This opens up the possibility to apply the qQMSA tools of ChemAdder to the HSQC signals and the 13C isotopomer distribution of each carbon of the 16 amino acids (i.e. the amino acids surviving the acid hydrolysis) can be obtained in less than 10 minutes. The QM models are field independent and the models obtained from the HSQC spectra measured at any field can be used as models for metabolic 13C labelling spectra measured at any other field.

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