The regulatory guidelines for dietary supplements stipulate that manufacturers provide verification that all products meet established identity, purity, strength, and composition requirements. The evaluation of botanical extracts and dietary supplements using NMR spectroscopy provides researchers with a flexible and powerful tool to comply with regulatory requirements. The intrinsic quantitative nature of NMR is increasingly exploited in areas ranging from complex mixture analysis as in food extracts. Complex NMR spectra are more common than not, and therefore, extraction of quantitative information generally involves significant prior knowledge and/or operator interaction to deconvolute peaks of interest.

We present an algorithm that achieves a Complete Reduction to Amplitude Frequency Table (CRAFT) in an automated and highly time-efficient fashion – thus converting the FID to a frequency-amplitude table. CRAFT tables can be used further for data mining of quantitative information using fingerprint chemical shifts of compounds of interest and/or statistical analysis of modulation of chemical quantity in a biological study (metabolomics). CRAFT approach is quantitative to very low concentrations even in complex mixtures.

Three commercially available dietary supplements containing soybean extract were investigated using $^1$H, $^{13}$C and Pure-shift 1D NMR spectroscopy. The spectra were analyzed using CRAFT. The basic principle behind the CRAFT approach, its application to the soy supplements and its potential for high throughput targeted and untargeted metabolomics will be presented.