Nuclear Magnetic Resonance for Targeted Metabolomics and Biochemical Sensor

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ABSTRACT

NMR spectroscopy is quantitative, highly reproducible, non-selective and non-destructive. However, NMR costs and complexity hinder a use as point-of-care and biochemical sensor instrumentation. Low field NMR (LF-NMR) is an inexpensive and low footprint technique to obtain physical, chemical, electronic and structural information on small molecules, but suffers from poor spectral dispersion, especially when applied to the analysis of mixtures. Subspectral editing employing optimal control pulses is a suitable approach to cope with the severe signal superpositions in complex mixture spectra at low field.

We have calculated the optimal control pulse shapes at 0.5 T NMR frequency using the Krotov algorithm. Downsizing the complexity of the algorithm from exponential to polynomial is shown to be possible by using a system approach with each system corresponding to a (small) molecule. In this way compound selective excitation pulses can be calculated. The signals of substructures of the cyclopentenone molecule were excited using optimal control pulses calculated by the Krotov algorithm demonstrating the feasibility of subspectral editing. Likewise, for a mixture of benzoic acid and alanine, editing of the signals of either benzoic acid or alanine employing optimal control pulses was shown to be possible.

The obtained results are promising and can be extended to the targeted analysis of complex mixtures such as biofluids or metabolic samples at low field strengths opening access for benchtop NMR to point of care settings. Moreover, the LF-NMR was improved to allow a unique detection and reliable quantification of metabolites in biofluids like blood, urine, cerebrospinal fluid, or even tissue. In contrast to standard large scale NMR equipment the portable LF-NMR allows for an analysis of the chemical composition of biofluid samples directly at the patient (point-of-care).

LF-NMR can be freely programmable for detecting and detecting and sensing sets of small molecules which deliver information on the health status of a person. Such an analytical tool would be useful for the prediction, diagnosis, monitoring and prognosis of diseases, and for supervision of therapeutic interventions.