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Using Filter Diagonalization Method to Process HR-MAS Spectra of Cancer Cells

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High-resolution magic angle spinning (HR-MAS) has been a promising tool to study metabolic profile of intact cancer cells and tissues. Although MAS technique strongly improves the spectra resolution of small molecules, it is not fast enough to reduce the line width of large molecules and assemblies signals. Therefore, they have been eliminated by a T_2 filter, based on Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence. Moreover, HR-MAS experiments with T_2 filter have to be preceded by water suppression procedure to avoid signal overlap and dynamic range problems. Although most of the HR-MAS experiments are focused in sharp signals of small molecules, information contained in broad signals may also be relevant. Despite the great success of this methodology, other techniques such as Filter Diagonalization Method (FDM) can be applied to the same purpose. In essence, FDM is a parametric non-linear method for fitting time-domain signals. Among other practical applications, the FDM has been recently used to selectively remove uninterested and corrupted solvent broad signals from complex NMR spectra without disturbing overlap or nearby narrower signals. They have shown that FDM can efficiently model broad signals in time domain for posterior subtraction from the original transient signal, resulting in an objective separation of the underlying structured spectrum. In this work we describe that the procedures of water suppression and T_2 or diffusing filters are unnecessary steps when the FDM is used to process the full time domain HR-MAS NMR signals obtained from breast cancer cells. Results demonstrate the efficiency of the FDM post-acquisition processing to obtain high resolution ^{1}H NMR spectra of heterogeneous biological materials, like cancer cells, even by using HR-MAS probe without water suppression and T_2 filter.