Simulation strategy for generating realistic NMR data

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Nuclear Magnetic Resonance (NMR) spectroscopy is a tool which allows us to measure concentration of thousands of metabolites simultaneously in biofluids, cells and tissues. Spectral data produced by NMR technology, has special features in both technical noise and signal which are different from data produced by mass spectrometry, for example a metabolite can be represented by a single or multiple peaks, and the peak location can vary depending on chemical characteristics of the medium, such as pH. We discuss these and other problems arising in modelling NMR data and present simulation strategies to produce realistic NMR data using available information about NMR characteristics of metabolites.