Accessory publication

Composition of dissolved organic matter within a lacustrine environment

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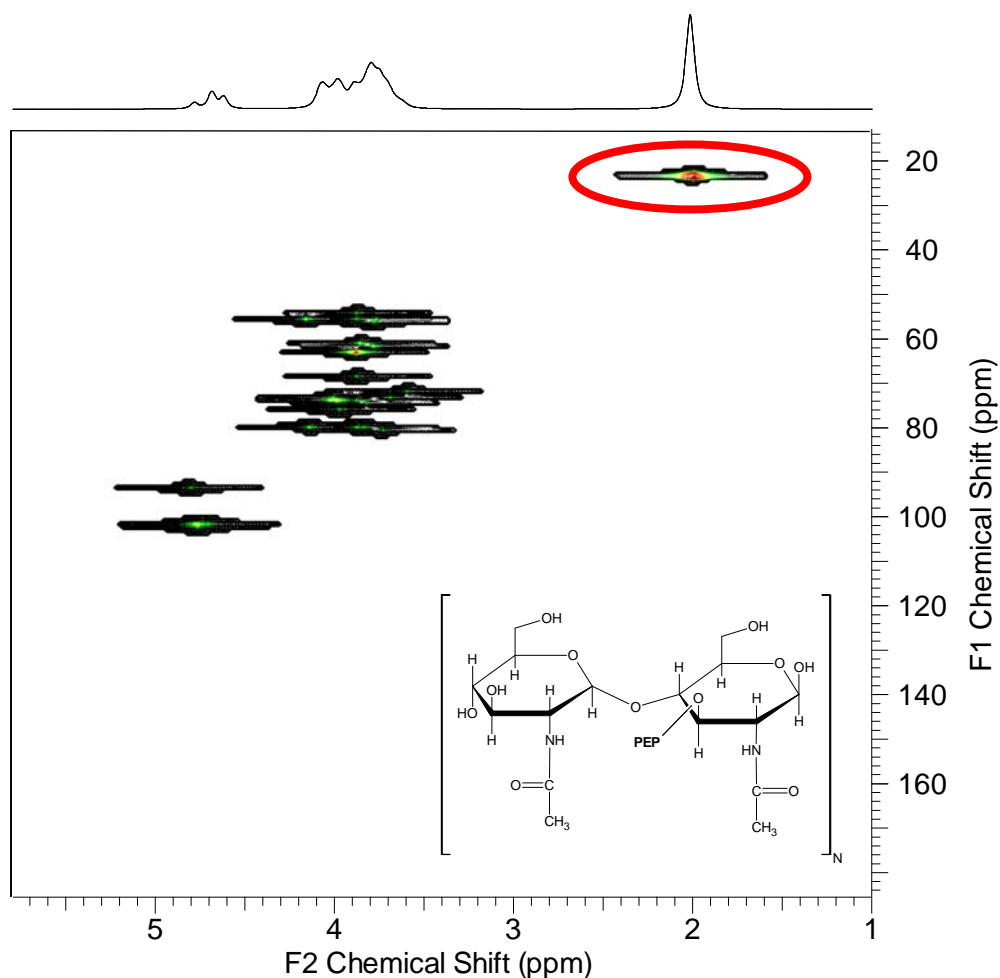
Fig. A1. Chemical shift prediction and 2-D ^{1}H–^{13}C spectral simulation of the backbone structure of peptidoglycan. PEP indicates the peptide branches that are not included in the prediction/simulation. Note: the chemical shifts of the carbohydrate units should be considered as rough approximations only as the chemical shifts of carbohydrates varies considerably with solution conditions (pH, concentration, salt background, etc.). The main purpose of the simulation is to demonstrate the strong CH$_3$–(C=O)–N resonance that is characteristic of peptidoglycan and is marked by a red oval. Spectral predictions were carried out using Advanced Chemistry Development's ACD/SpecManager and ACD/2-D NMR Predictor using Neural Network Prediction algorithms (version 12.01) and water as the solvent. Parameters used for prediction including spectral resolution, and base frequency were chosen to match those of the real datasets as closely as possible.