Isotope Labeling with $^{13}\text{C}$-Iodomethane in Comparison with Deuterated Iodomethane for the Analysis of Methyl Patterns in Methylcellulose

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Cellulose ethers are on a quantity basis the most important cellulose derivatives. The annual production amounts to 650,000 tons. Concerning their rheological, emulsifying, thickening and film-forming properties, they have a wide field of application in food-, cosmetics-, pharmacy- as well as textile and building material industry. The characteristics significantly depend on the molar mass, chemistry of substituents as well as degree of substitution (DP) and substitution pattern on various hierarchical levels.

Presently, the determination of methyl patterns in methylcellulose is carried out using ESI-MS after peralkylation with deuterated iodomethane and partial hydrolysis to a complex mixture of oligosaccharides (OS). In ESI-MS the ionization efficiency depends on many factors of the analyte structure (e.g. number and position of substituents → complexing properties [1], surface activity, volatility, molecular weight). The idea of peralkylation of the free hydroxyl groups is to unify the structure of the OS with the same DP, and thus to minimize the influence of the analyte structure on the ionization efficiency.

However, peralkylation with deuterated iodomethane has two sticking points: CD₃ is more hydrophobic and volatile compared to CH₃, so that discrimination effects can be observed at higher DPs [2]. Therefore, we investigated whether peralkylation with $^{13}\text{C}$-labeled iodomethane can superiorly compensate structural differences in the analysis of methyl patterns in methylcellulose. $^{13}\text{C}$-Me as isotopic label satisfies the chemical and physical requirements much better. But, due to the naturally occurring $^{13}\text{C}$ content, the signals have to be corrected mathematically. Studies if this correction can be done with sufficient accuracy are presented and compared to CD₃-peralkylation.

References