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Data Article

Two-dimensional NMR data of a series of methylcellulose with different degrees of substitution

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A R T I C L E I N F O

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A B S T R A C T

This article contains two-dimensional (2D) NMR experimental data for a series of methylcellulose (MC) with different substitution degrees (DS), obtained by the Bruker BioSpin 500 MHz NMR spectrometer (Germany). The data facilitated the ^{1}H and ^{13}C chemical shifts of eight anhydroglucose units (AGUs) comprising MC chains–unsubstituted, 2-mono-, 3-mono-, 6-mono-, 2,3-di-, 2,6-di-, 3,6-di-, and 2,3,6-tri-substituted AGUs. Data include analyzed the 2D NMR spectra of the MC samples, which are related to the subject of an article in *Carbohydrate Polymers*, entitled "NMR characterization of methylcellulose: Chemical shift assignment and mole fraction of monomers in the polymer chains" (Kon et al., 2017) [1]. These data can be very helpful to assign the ^{1}H and ^{13}C chemical shifts of the other cellulose derivatives, especially cellulose ethers.

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Specifications table

Subject area	*Chemistry*
More specific subject area	*Structural analysis*
Type of data	*NMR spectra*

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How data was acquired	*NMR, Bruker BioSpin AVIII* 500 MHz *spectrometer equipped with a Bruker BioSpin z-gradient dual-resonance BBFO probe (*5 mm*).*
Data format	*Analyzed*
Experimental factors	*About 35* mg *of each sample dissolved in 700 μL of 99.9% dimethylsulfoxide (DMSO)-d_6* containing 0.03% tetramethylsilane (TMS).
Experimental features	*All NMR experiments were performed at 363* K.
Data source location	*National Institute of Technology, Tomakomai College, Nishikioka 443, Tomakomai, Hokkaido 0591275, Japan*
Data accessibility	*Data are with this article.*

Value of the data

- The following data detail NMR characterization of a MC samples with different DS.
- The NMR data can be helpful to assign the chemical shifts of AGUs comprising other cellulose derivatives.
- NMR parameters used for the obtained data can be useful for structural characterization of complex polysaccharides.

1. Data

Cellulose is a linear 1,4-β-D-glucan with three hydroxyl groups per anhydroglucose units (AGU). Each AGU contains three hydroxyl groups at the 2, 3, and 6 positions. In the case of methylcellulose (MC), substitution can occur at theses hydroxyl groups, resulting in the formation of 8 different AGUs in the structure except for total degree of substitution (DS) of 3, namely, unsubstituted, 2-mono-, 3-mono-, 6-mono-, 2,3-di-, 2,6-di-, 3,6-di-, and 2,3,6-tri-substituted AGUs (Fig. 1). The complexity of

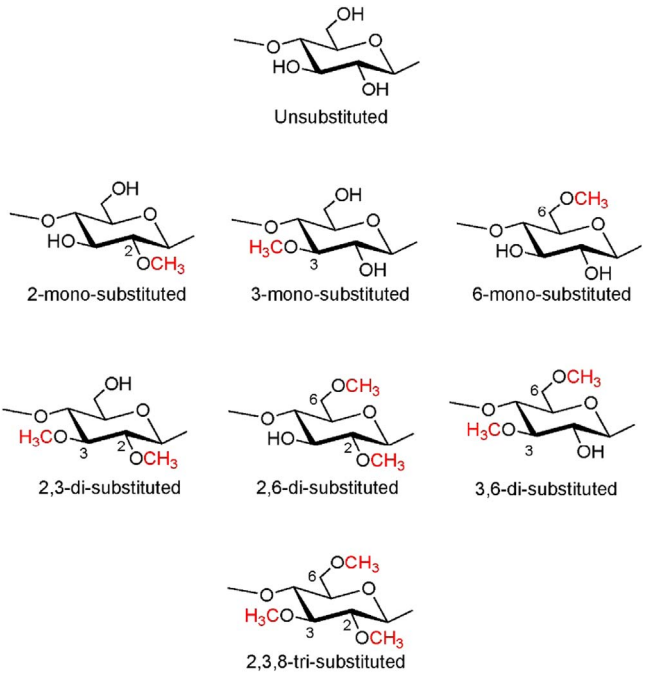

Fig. 1. Eight anhydroglucose units (AGUs) comprising methylcellulose (MC) chains.

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