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Data Article

Two-dimensional NMR data of a water-soluble β-(1→3, 1→6)-glucan from *Aureobasidium pullulans* and schizophyllan from *Schizophyllum commune*

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ABSTRACT

This article contains two-dimensional (2D) NMR experimental data, obtained by the Bruker BioSpin 500 MHz NMR spectrometer (Germany) which can used for the determination of primary structures of schizophyllan from *Schizophyllum commune* (SPG) and a water-soluble β-(1→3, 1→6)-glucan from *Aureobasidium pullulans*. Data include analyzed the 2D NMR spectra of these β-glucans, which are related to the subject of an article in *Carbohydrate Polymers*, entitled "NMR spectroscopic structural characterization of a water-soluble β-(1→3, 1→6)-glucan from

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A. pullulans" (Kono et al., 2017) [1]. Data can help to assign the ^{1}H and ^{13}C chemical shifts of the structurally complex polysaccharides.

Specifications Table

Subject area	*Chemistry*
More specific subject area	*Structural analysis*
Type of data	*NMR spectra*
How data was acquired	*NMR, Bruker BioSpin AVIII 500 MHz spectrometer*
Data format	*Analyzed*
Experimental factors	*About 30 mg of each sample dissolved in 600 μL of 99.9% dimethylsulfoxide (DMSO)-d_6.*
Experimental features	*All NMR experiments were performed at 363 K.*
Data source location	*National Institute of Technology, Tomakomai College, Nishikioka 443, Tomakomai, Hokkaido 059 1275, Japan*
Data accessibility	*Data are with this article.*

Value of the data

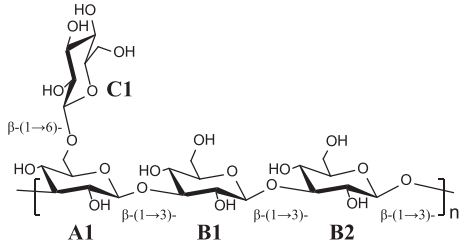
- The following data detail NMR characterization of a novel water-soluble β-(1→3, 1→6)-glucan and schizophyllan from *Schizophyllum commune.*
- The NMR data can be helpful to estimate the branching patterns of other β-glucans.
- NMR parameters for the data can be useful for structural characterization of complex polysaccharides.

1. Data

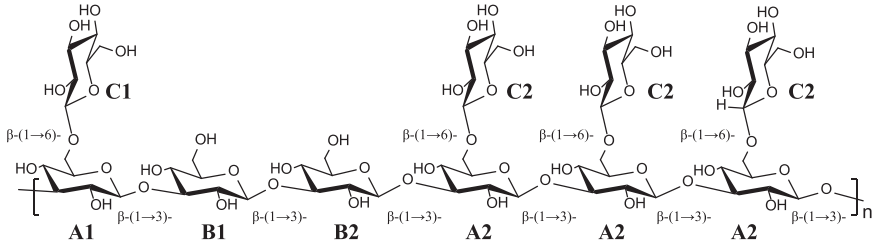
The presented data include 2D NMR spectra of schizophyllan from *Schizophyllum commune* (SPG) and a water-soluble β-(1→3, 1→6)-glucan from *Aureobasidium pullulans* (*A. pullulans*) whose primary structures are shown in Fig. 1. ^{1}H–^{13}C heteronuclear single quantum coherence (HSQC), 2D ^{1}H–^{13}C heteronuclear multiple-bond correlation (HMBC), and 2D ^{1}H–^{1}H rotating frame Overhauser effect spectroscopy (ROESY) spectra of SPG are shown in Figs. 2–4, and those of the water-soluble *A. pullulans* β-(1→3, 1→6)-glucan are in Figs. 5–7, respectively.

2. Experimental design, materials and methods

The experiment's planning, design, and data processing correspond to the protocol given in Refs. [1,2].



Schizophyllan from *Schizophyllum commune* (SPG)



A water-soluble β-(1→3, 1→6)-glucan from *Aureobasidium pullulans*

Fig. 1. Primary structures of schizophyllan (SPG) and the water-soluble β-(1→3, 1→6)-glucan from *A. pullulans*. The **A1**, **B1**, **B2**, and **C1** residues in SPG and **A1**, **A2**, **B1**, **B2**, **C1**, and **C2** residues in the β-(1→3, 1→6)-glucan are magnetically inequivalent in their structures.

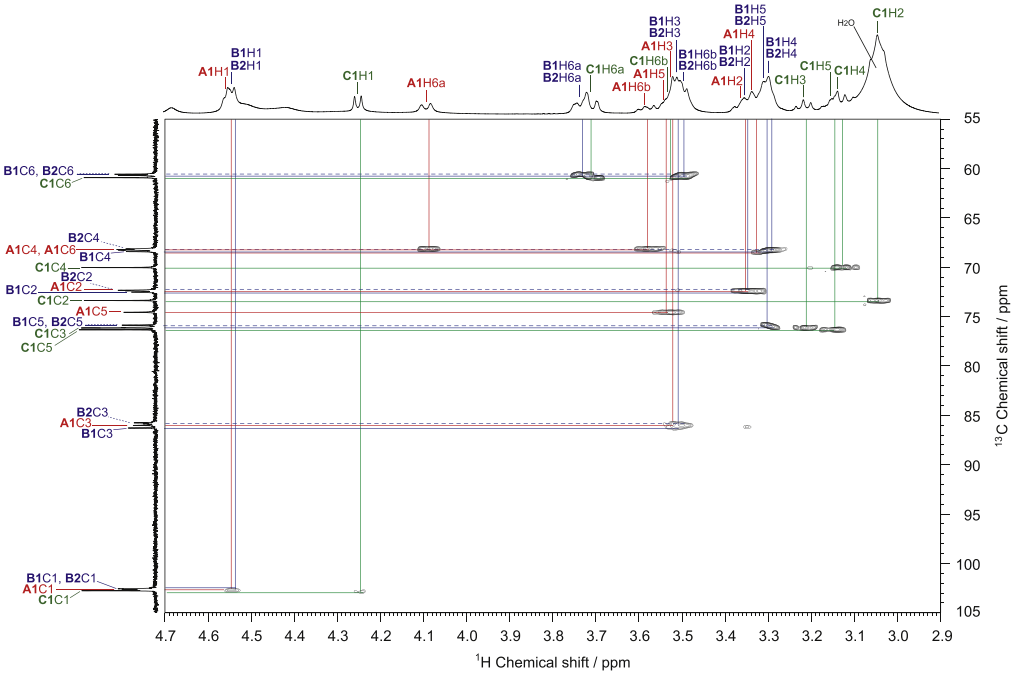


Fig. 2. HSQC spectrum of SPG in DMSO-d_6 at 363 K. The vicinal ^{1}H–^{13}C spin couplings of the **A1**, **B1**, **B2**, and **C1** residues in SPG (Fig. 1) are denoted by solid red, solid and dashed blue, and solid green lines, respectively. ^{1}H and ^{13}C NMR spectra of SPG are shown in horizontal and vertical axes in the HSQC spectrum, respectively, and the ^{1}H and ^{13}C resonance assignments are indicated in the ^{1}H and ^{13}C spectra.

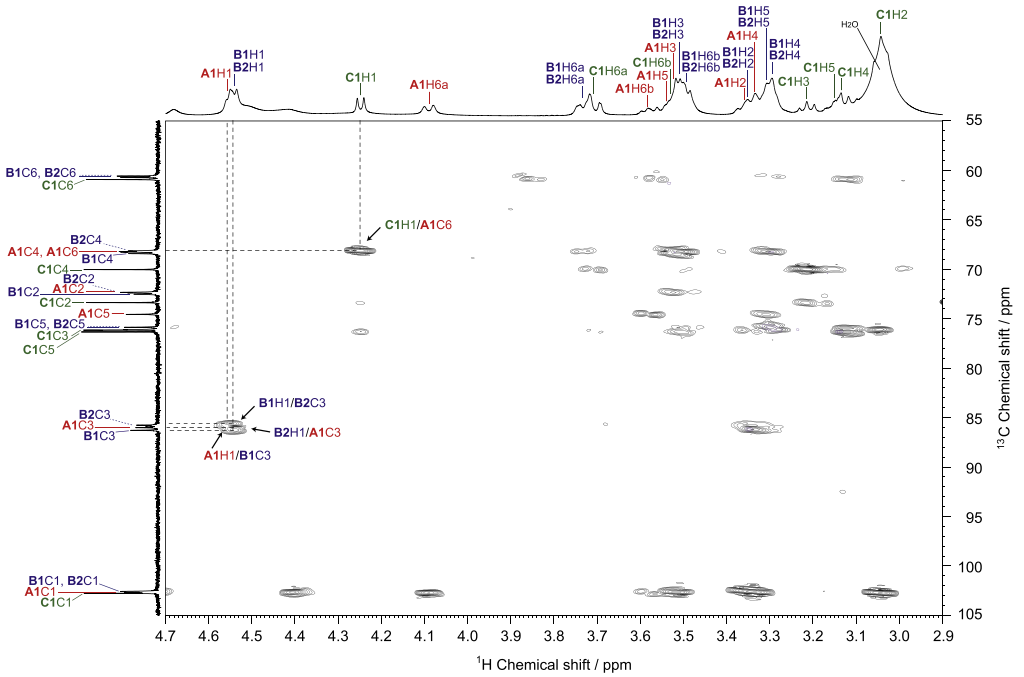


Fig. 3. HMBC spectrum of SPG in DMSO-d_6 at 363 K. The arrows indicate the interresidual correlations between **A1**H1–**B1**C3, **B1**H1–**B2**C3, **B2**H1–**A3**C3, and **C1**H1–**A1**C6 via glycosidic bonds.

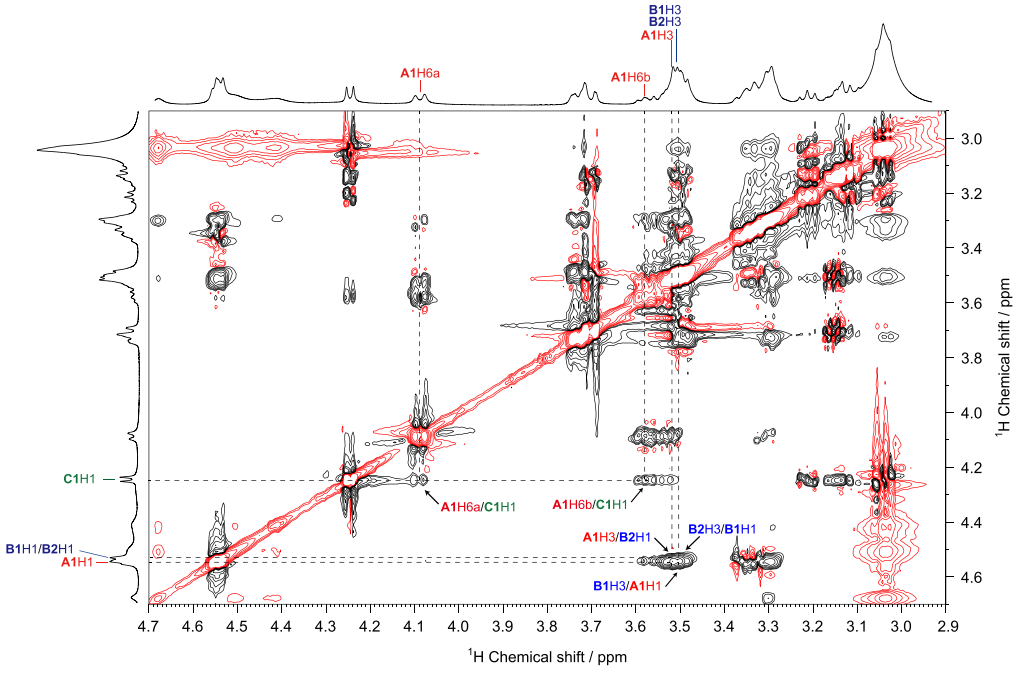


Fig. 4. ROESY spectrum of SPG in DMSO-d_6 at 363 K. The arrows indicate the interresidual correlations between **B1**H3–**A1**H1, **A1**H3–**B2**H1, **B2**H3–**B1**H1, **A1**H6a–**C1**H1, and **A1**H6b–**C1**H1 via glycosidic bonds.

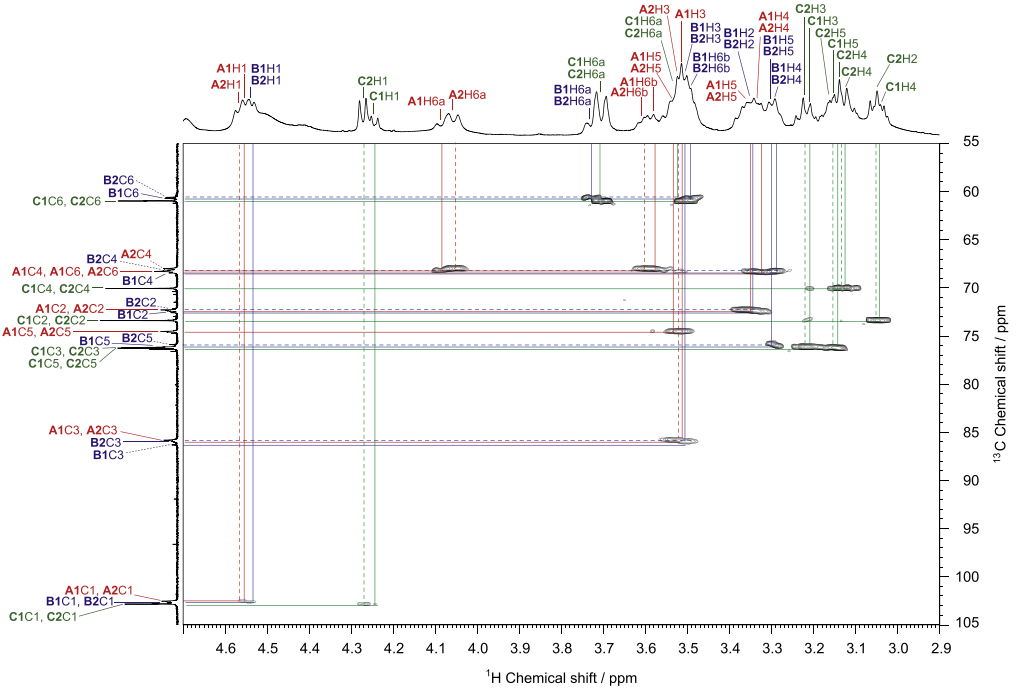


Fig. 5. HSQC spectrum of the water-soluble β-(1→3, 1→6)-glucan from *A. pullulans* in DMSO-d_6 at 363 K. The vicinal ^{1}H–^{13}C spin couplings of the **A1**, **A2**, **B1**, **B2**, **C1**, and **C2** residues in the β-(1→3, 1→6)-glucan (Fig. 1) are denoted by solid and dashed red, solid and dashed blue, and solid and dashed green lines, respectively. ^{1}H and ^{13}C NMR spectra of the β-(1→3, 1→6)-glucan are shown in horizontal and vertical axes in the HSQC spectrum, respectively, and the ^{1}H and ^{13}C resonance assignments are indicated in the ^{1}H and ^{13}C spectra.

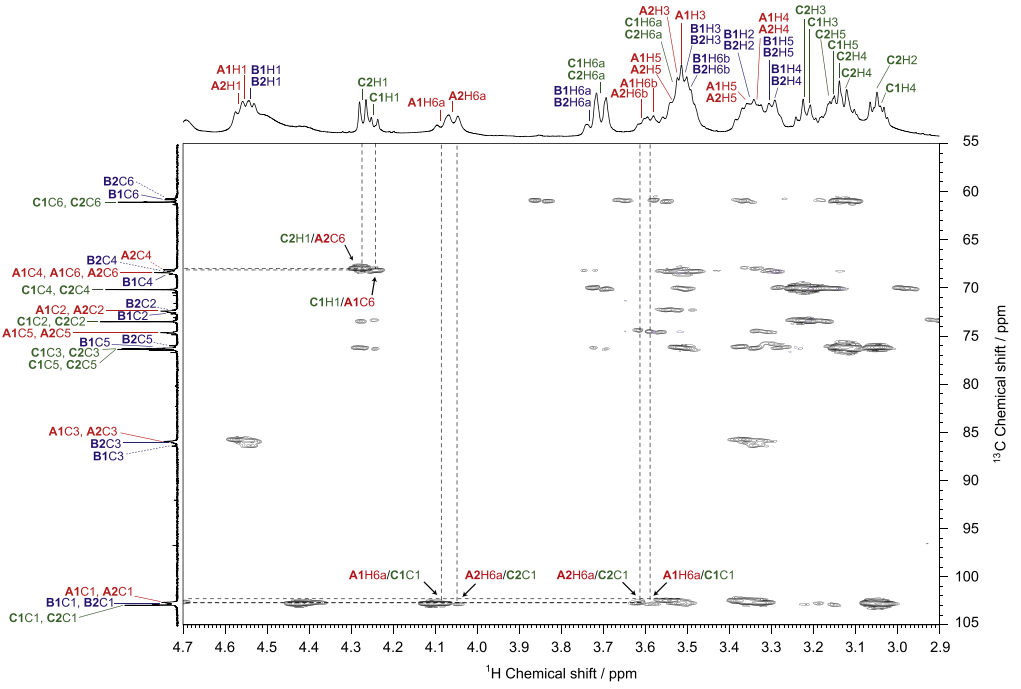


Fig. 6. HMBC spectrum of the water-soluble β-(1→3, 1→6)-glucan from *A. pullulans* in DMSO-d_6 at 363 K. The arrows indicate the inter-residual correlations between **C1**C1–**A1**H6a, **C1**C1–**A1**H6b, **C2**C1–**A2**H6a, **C2**C1–**A2**H6b, **C1**H1–**A1**C6, and **C2**H1–**A2**C6 via glycosidic bonds.

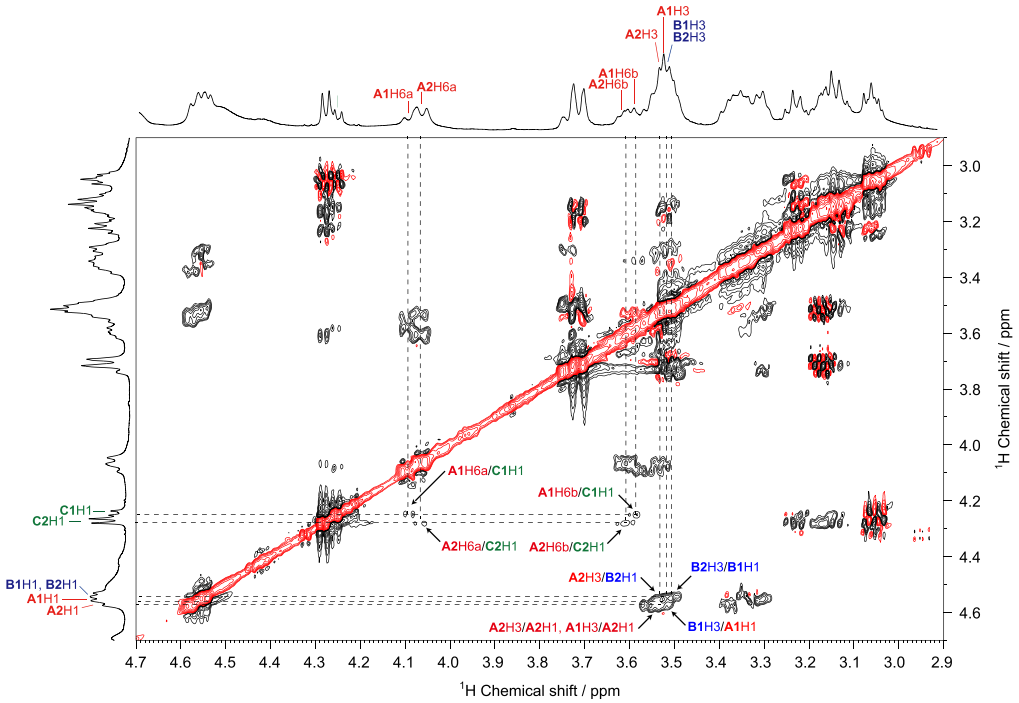


Fig. 7. ROESY spectrum of the water-soluble β-(1→3, 1→6)-glucan from *A. pullulans* in DMSO-d_6 at 363 K. The arrows indicate the interresidual correlations between **A2**H3–**B2**H1, **A1**H3–**A2**H1, **B1**H3–**A1**H1, **A2**H3–**B2**H1, **B2**H3–**B1**H1, **A2**H6a–**C2**H1, **A2**H6b–**C2**H1, **A1**H6a–**C1**H1, and **A1**H6b–**C1**H1 via glycosidic bonds.

2.1. Samples

SPG was purchased from InvivoGen (USA). The water-soluble *A. pullulans* β-(1→3, 1→6)-glucan was prepared according to a previously reported method [1,2].

2.2. Description of the NMR experiments

Each sample was dissolved in 600 μL of DMSO-d_6 (99.9% isotropic purity, Sigma-Aldrich (USA)). All NMR spectra were recorded on a Bruker AVIII 500 MHz spectrometer at 363 K. HSQC data were acquired on a 2048 × 256-point matrix for the full spectrum, with 96 scans per increment, and the interpulse delay which corresponded to 1/4 J_{CH} was set to 3.44 ms. HMBC) data were acquired on a 1024 × 256-point matrix for the full spectrum, with 128 scans per increment, and the delay time for the evolution was set to 62.5 ms. ROESY data were acquired on a 2048 × 256-point matrix for the full spectrum with 64 scans per increment, and the mixing time was 200 ms. The repetition time of each 2D NMR experiment was 2 s, and all 2D NMR data were zero-filled to 2k in both dimensions prior to Fourier transformation. ^{1}H and ^{13}C chemical shifts were calibrated using the methyl resonances of DMSO at 2.52 ppm for ^{1}H and 39.52 ppm for ^{13}C.

Acknowledgements

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[2] K. Hirabayashi, N. Kondo, S. Hayashi, Characterization and enzymatic hydrolysis of hydrothermally treated β-1,3–1,6-glucan from *Aureobasidium pullulans*, World J. Microbiol. Biotechnol. 32 (2016) 206–212.