SUPPORTING INFORMATION FOR

Specific binding of a naturally occurring amyloidogenic fragment of *Streptococcus mutans* adhesin P1 to intact P1 on the cell surface characterized by solid state NMR spectroscopy

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Figure S1. Dot blot of NG8 cell wall after varying bead beater cycles (1 to 10) along with PC3370 cell wall as a control. The primary antibodies used are 1-6F (lower panel, recognizes the head region of P1) and 6-8C (top panel, recognizes the C-terminus of P1). We note levels of P1 are approximately the same regardless of the number of cycles, but that the yield of cell wall fragments increases dramatically as we go from <5 to >5 cycles. This mechanical treatment also increases the exposure of the P1 C-terminal epitope recognized by 6-8C, as we have noted and characterized in previous work (Heim et al. 2015)

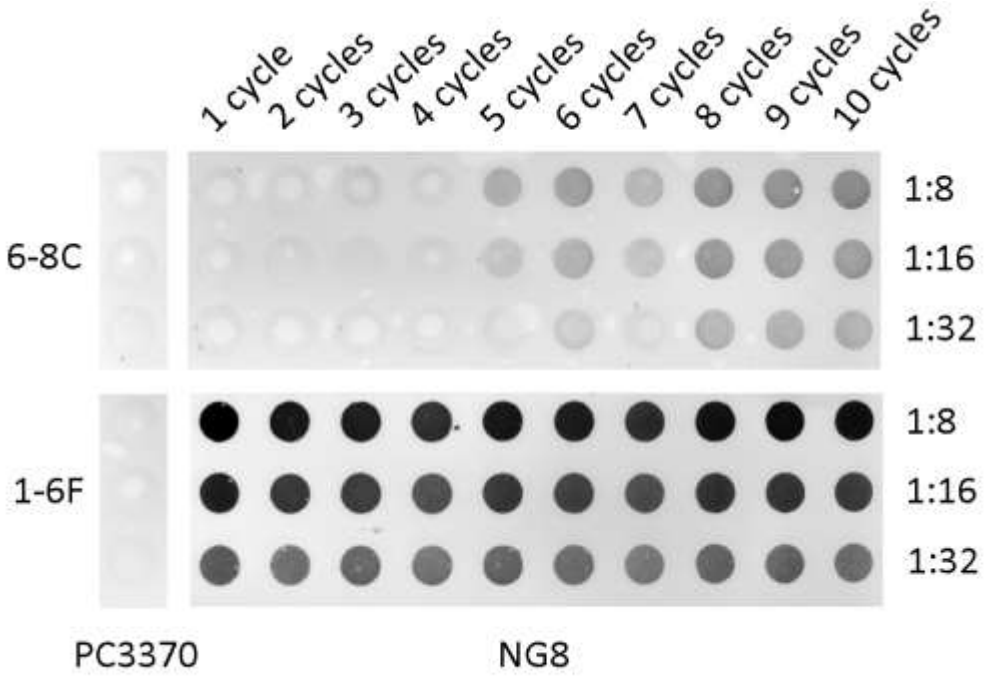

Figure S2. Comparison of one-dimensional ^{13}C CPMAS and DPMAS experiments on the NG8 cell wall sample. Both spectra show 10k scans collected at 4 °C and a MAS rate of 12 kHz. ^{13}C nuclei in the more dynamic region (such as protein side chains) experience less efficient polarization transfer than those in the more rigid regions. The overall retention of signals in the CPMAS spectrum is consistent with the limited motion of the peptidoglycan and attached proteins even at full hydration.

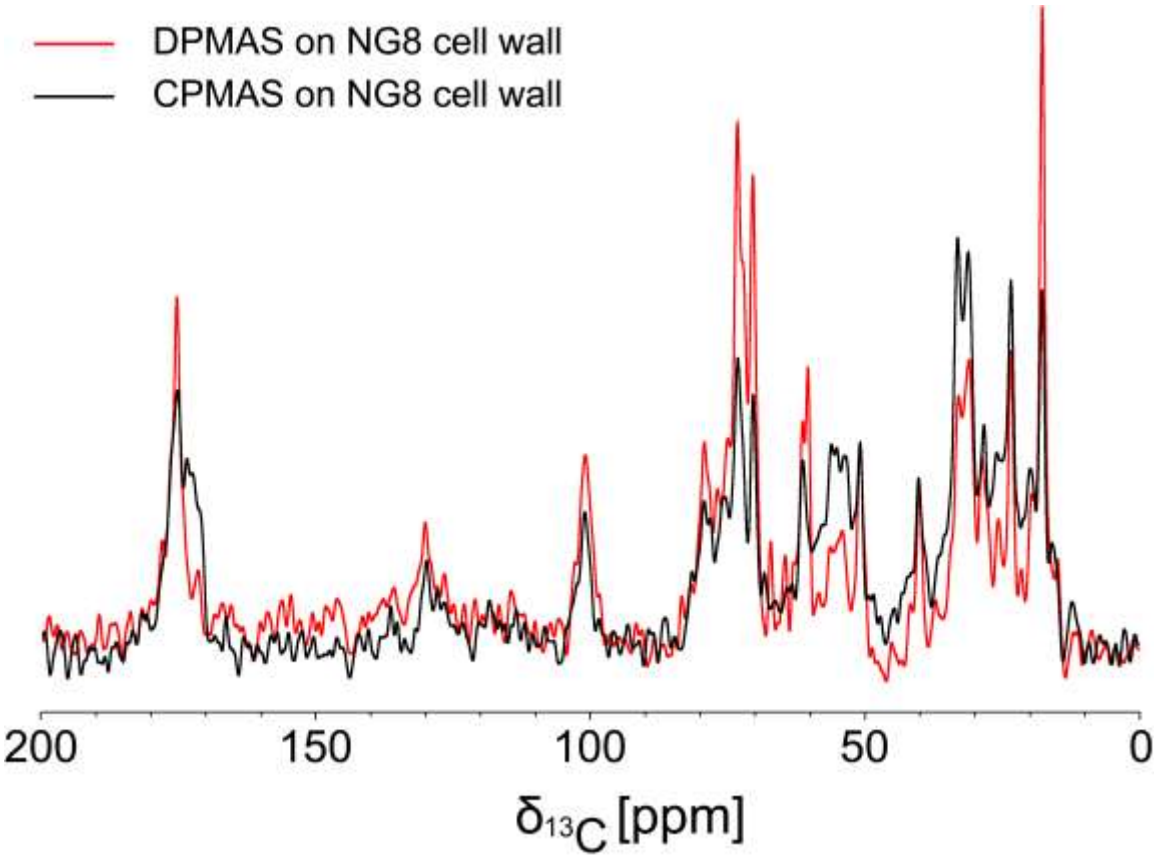

Figure S3. Comparison of NG8 whole cells and NG8 cell walls isolated after 3 bead beater cycles. Both CPMAS experiments were carried out at 500 MHz at -40 °C with a spinning rate of 12k Hz. 4k scans were collected for each of the experiments.

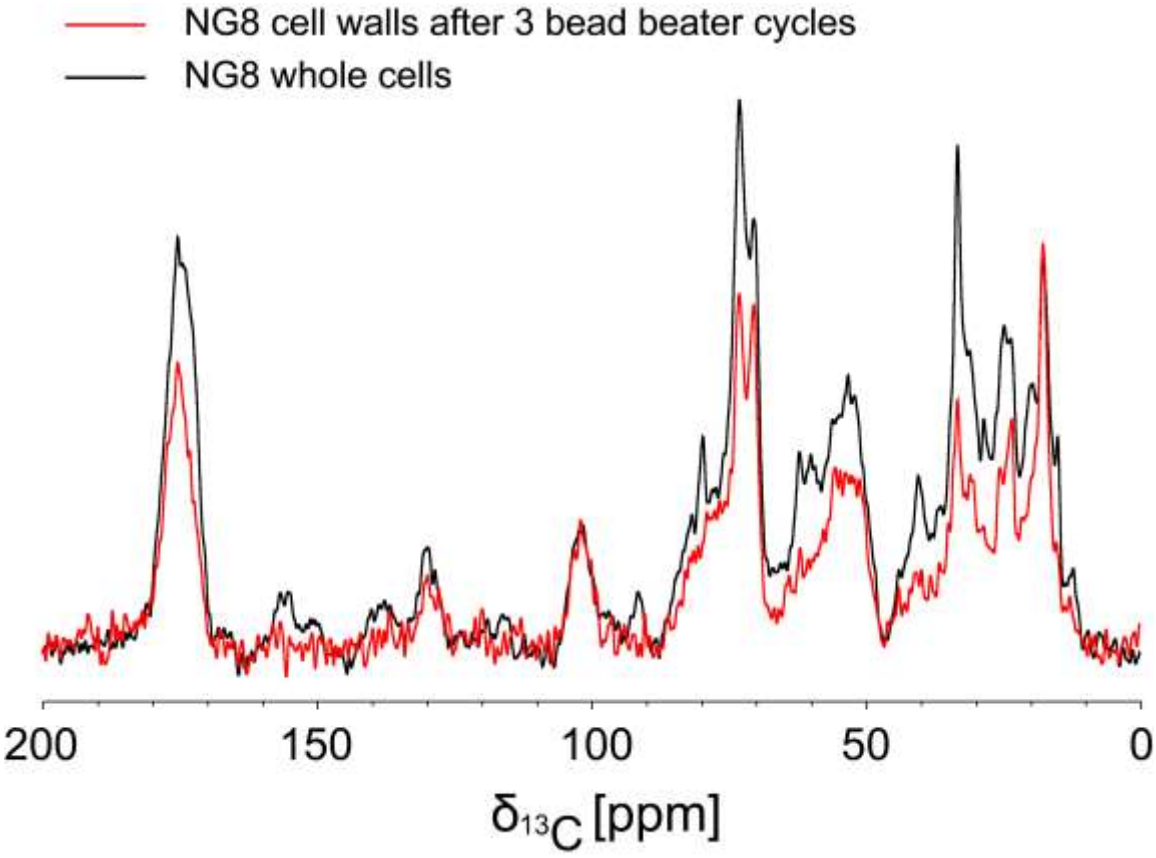

Figure S4. One-dimensional ^{13}C CPMAS spectra of PC3370 cell walls before (black) and after (red) SDS/trypsin treatment as well as the difference spectrum (blue) of the two. Both spectra show 10k scans collected at 4 °C and a MAS rate of 12 kHz. The peptidoglycan signals remain after treatment while protein signals are lost; observed loss of protein is similar to what was observed for NG8 cell walls (Figure 3).

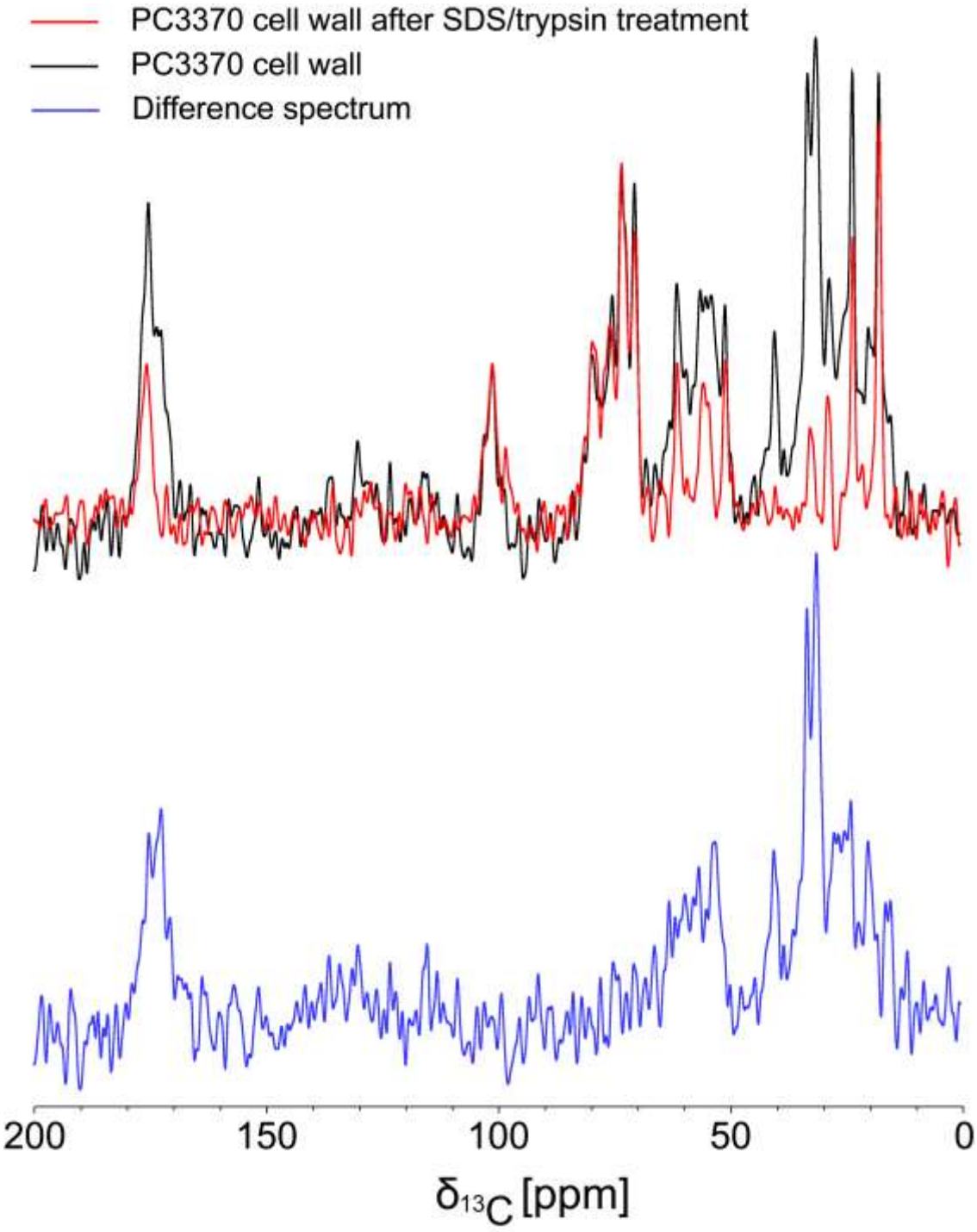

Figure S5. ^{13}C DPMAS spectra of NG8 untreated cell walls before (black) and after (red) the addition of ^{13}C enriched C123. The difference spectrum (blue) indicates binding of C123 to NG8 cell wall components (P1 in particular). The inset compares ^{13}C DPMAS spectra of NG8 cell wall (black) with PC3370 cell wall after the addition of ^{13}C enriched C123, showing no appreciable binding of C123 to PC3370 cell walls. All spectra show 10k scans collected at 4 °C and a MAS rate of 12 kHz. Signals in these spectra relative to CPMAS spectra in Figure 4 are consistent with limited C123 motion on binding P1.

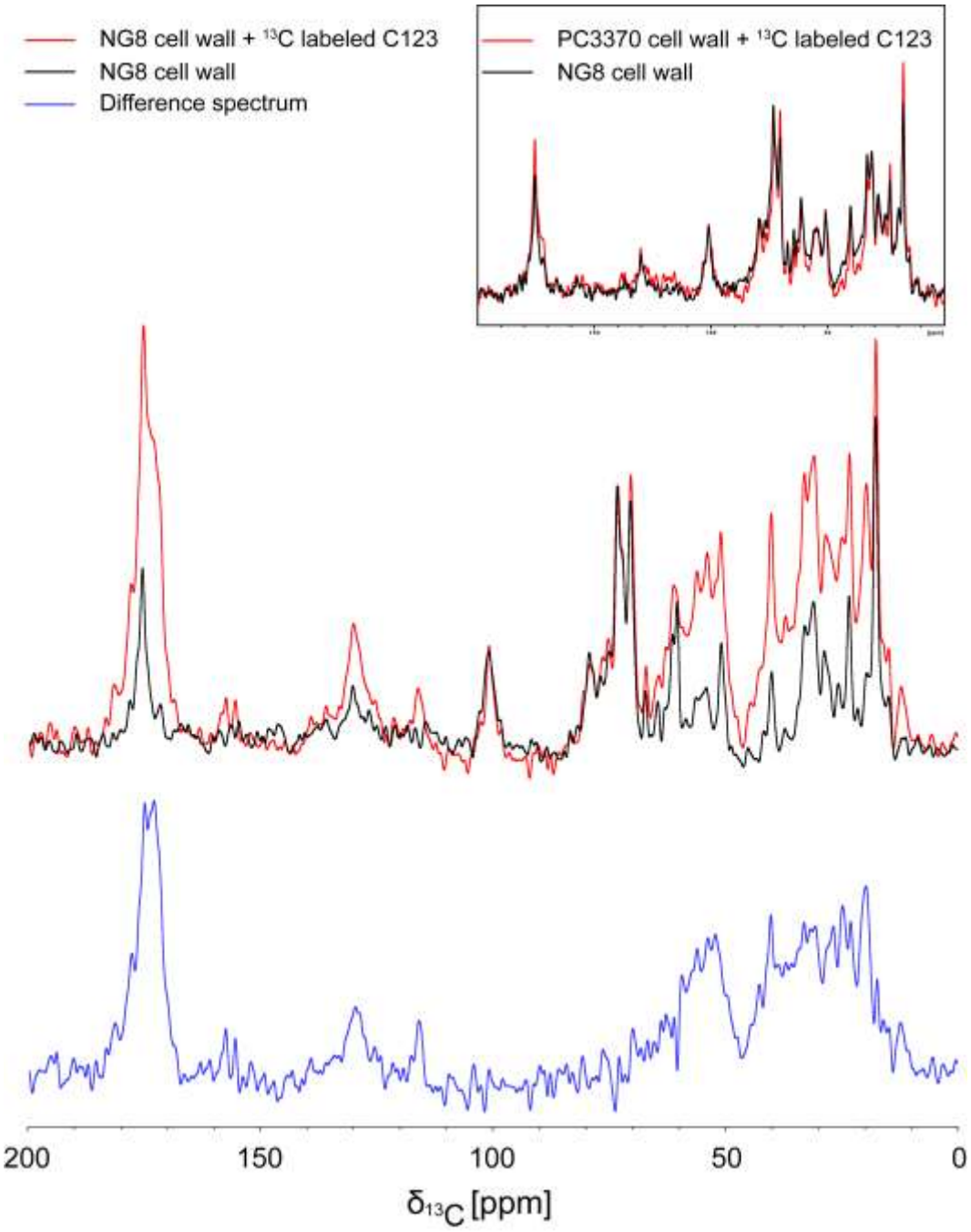

Figure S6. (Left) One-dimensional ^{13}C CPMAS spectra of SDS/trypsin treated NG8 cell walls before (black) and after (red) the addition of ^{13}C enriched C123 as well as the difference spectrum (blue) of the two. Both spectra show 10k scans collected at 4 °C and a MAS rate of 12 kHz. The signal intensities over the regions corresponding to protein resonances didn't change, indicating C123 did not bind to any cell wall component. Similar results are obtained for PC3370 cell walls (right).

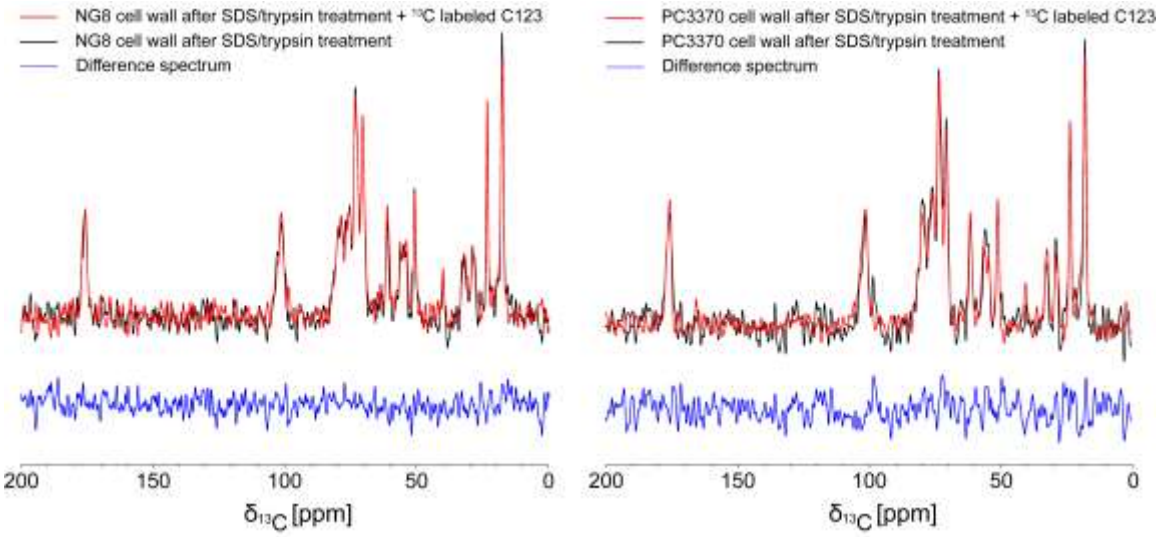

Figure S7. $^{13}C/^{15}N$ REDOR spectra of NG8 (left panel) and PC3370 (right panel) cell walls after the addition of ^{13}C enriched C123 and glutaraldehyde fixation. A difference spectrum (blue) was produced by subtracting the dephased S spectrum (black) from the S_0 control spectrum (red) for both samples. Both spectra show 8k scans collected at -5 °C and a MAS rate of 10 kHz.

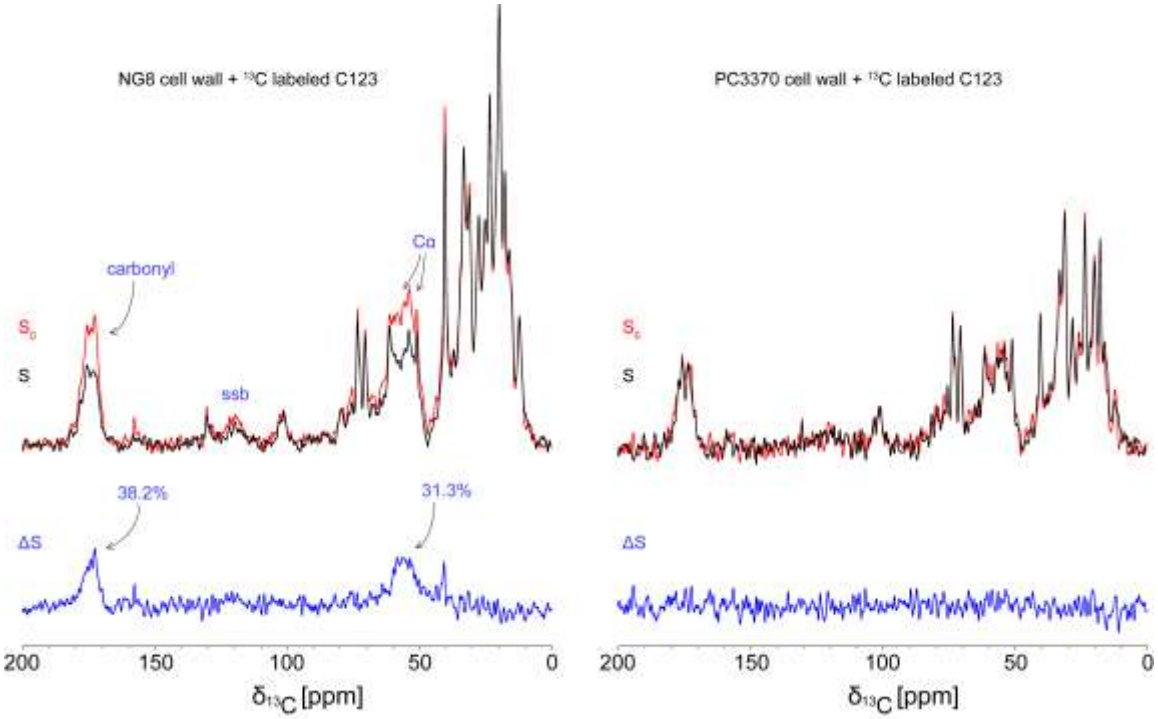

Figure S8. Comparison of NG8 cell walls after 3, 7 and 10 bead beater cycles. All CPMAS experiments were carried out at -40 °C with a spinning rate of 12k Hz.No appreciable differences in relative signal intensities are seen between the different sample preparations.

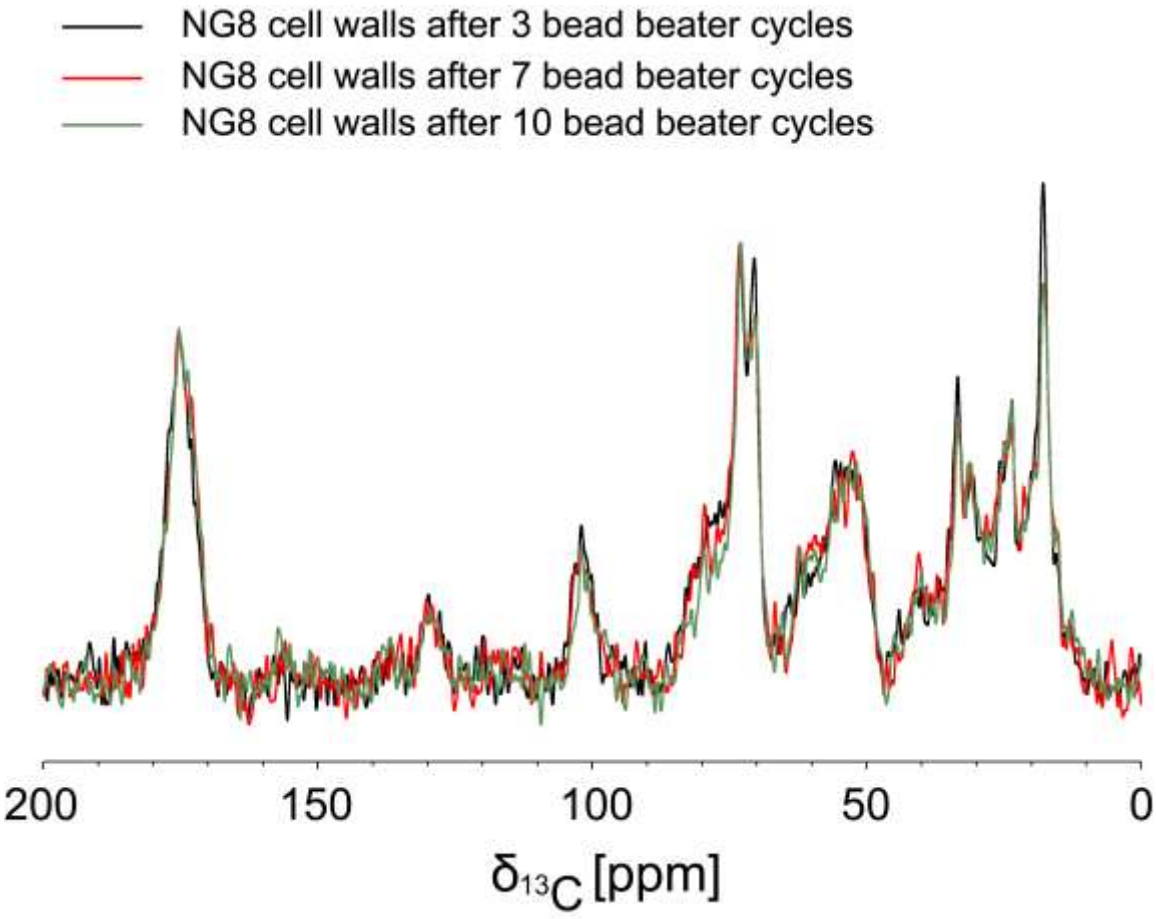

Figure S9. Protein-protein interactions were predicted by submitting the X-ray crystal structures of A3VP1 and C123 domains of P1 (PDB ID: 3IPK and 3QE5) to the PRISM webserver. The three highest scoring interactions are shown (from left to right) with scores of -8.35, -9.16, and -5.46.

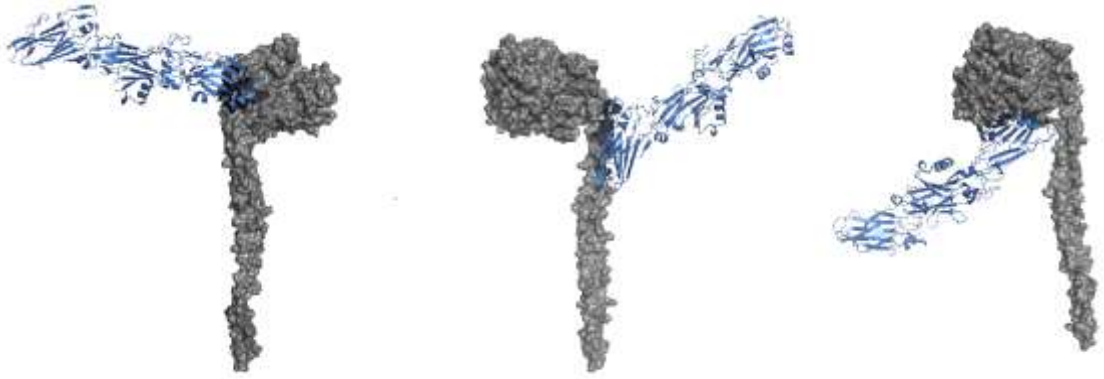

Table S1. Relative peak area integrations of carbonyl carbon and α carbon regions of the $^{13}C/^{15}N$ REDOR spectra (at 233 K) for NG8 cell wall after binding of ^{13}C enriched C123 and glutaraldehyde fixation.

	carbonyl carbon (170-180 ppm)	α carbon (50-58 ppm)
S0	1	1
S	0.18	0.25
ΔS	0.82	0.75