Supporting Information
Effect of oxidation on cellulose and water structure: a molecular dynamics simulation study

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The Supporting Information consists of root mean square deviation (RMSD) of the cellulose crystal coordinates calculated from the simulations (Figure S1), a zoom of main manuscript Figure 11 cellobionic acid (DP2ox) and cellohexaose (DP6) peak region, and the full chromatogram data set.

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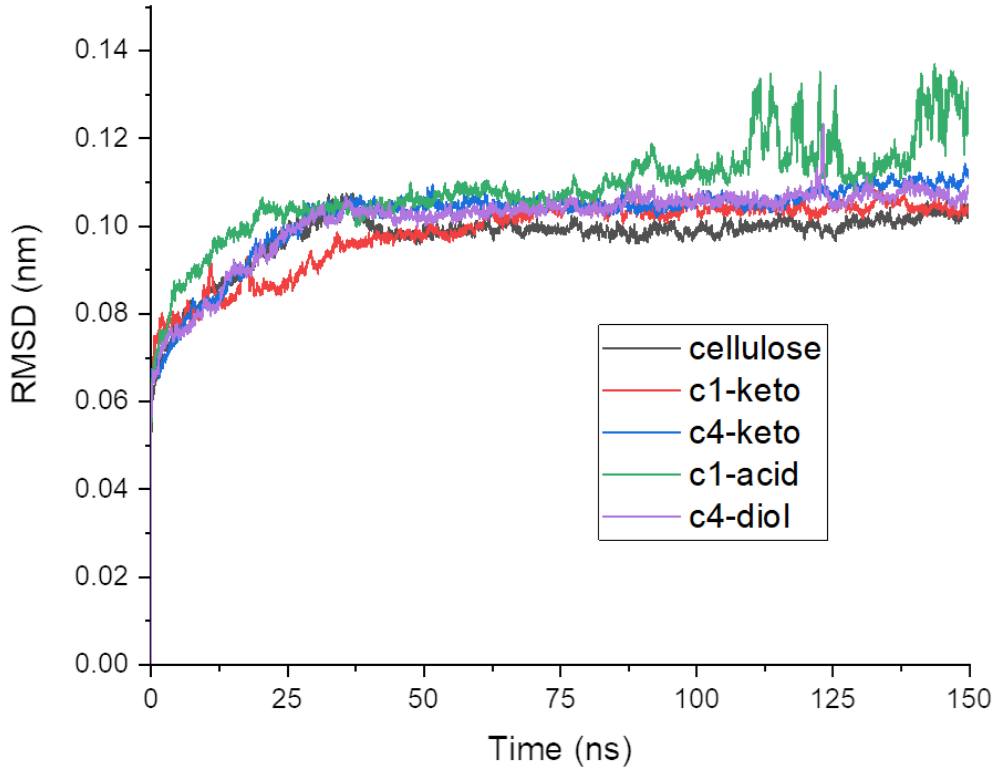

Figure S1: Root mean square deviation (RMSD) of intact and oxidized cellulose crystals in the molecular dynamics simulations.

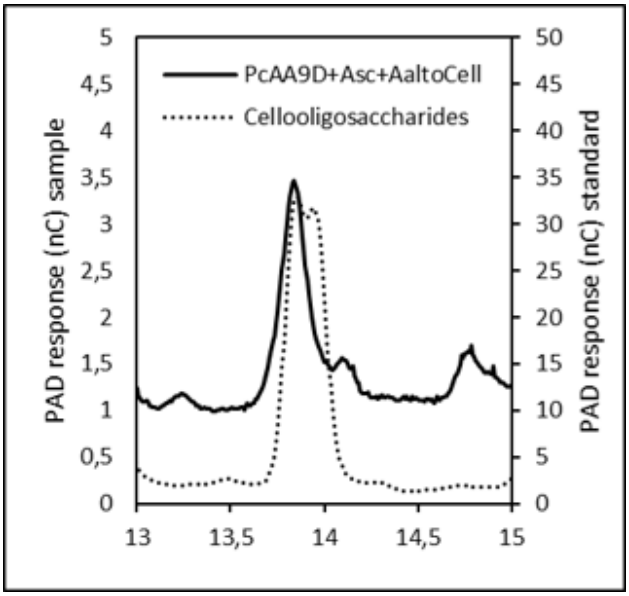

Figure S2: Zoom corresponding to main manuscript Figure 11 cellobionic acid (DP2ox) and cellohexaose (DP6) peak region.

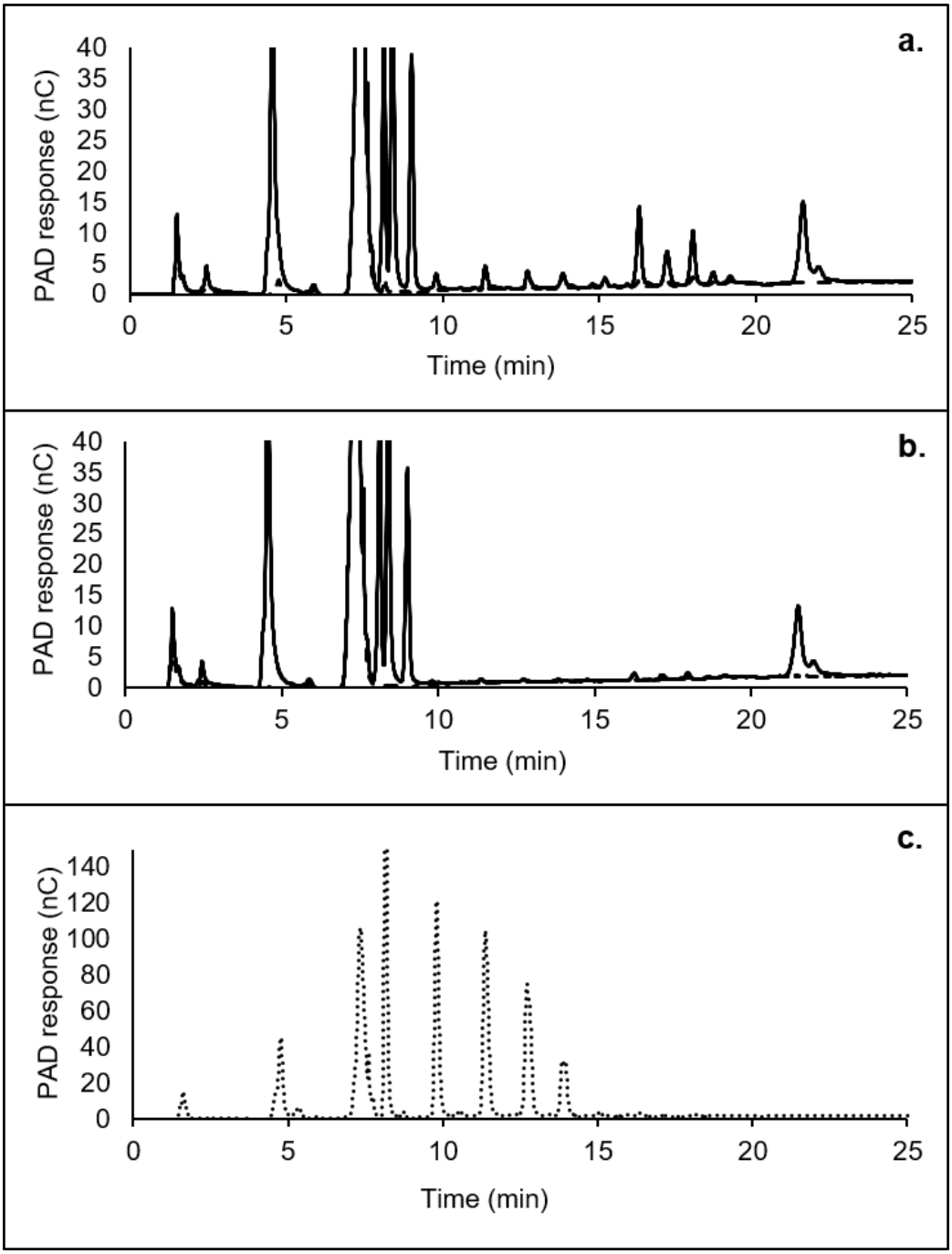

Figure S3: Full chromatogram data set.