

Supporting Information for “Effects of temperature, concentration, and isomer on the hydration structure in monosaccharide solutions”

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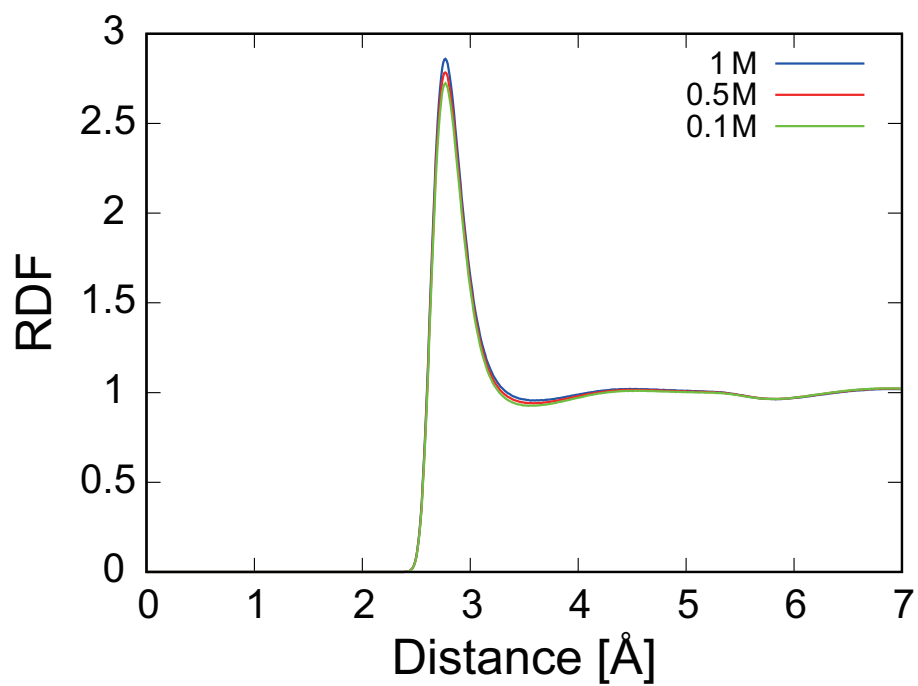


Figure S1: **RDFs of water oxygen-oxygen.** Green, red, and blue lines show α -D-glucose solution at 0.1, 0.5, and 1 M, respectively.

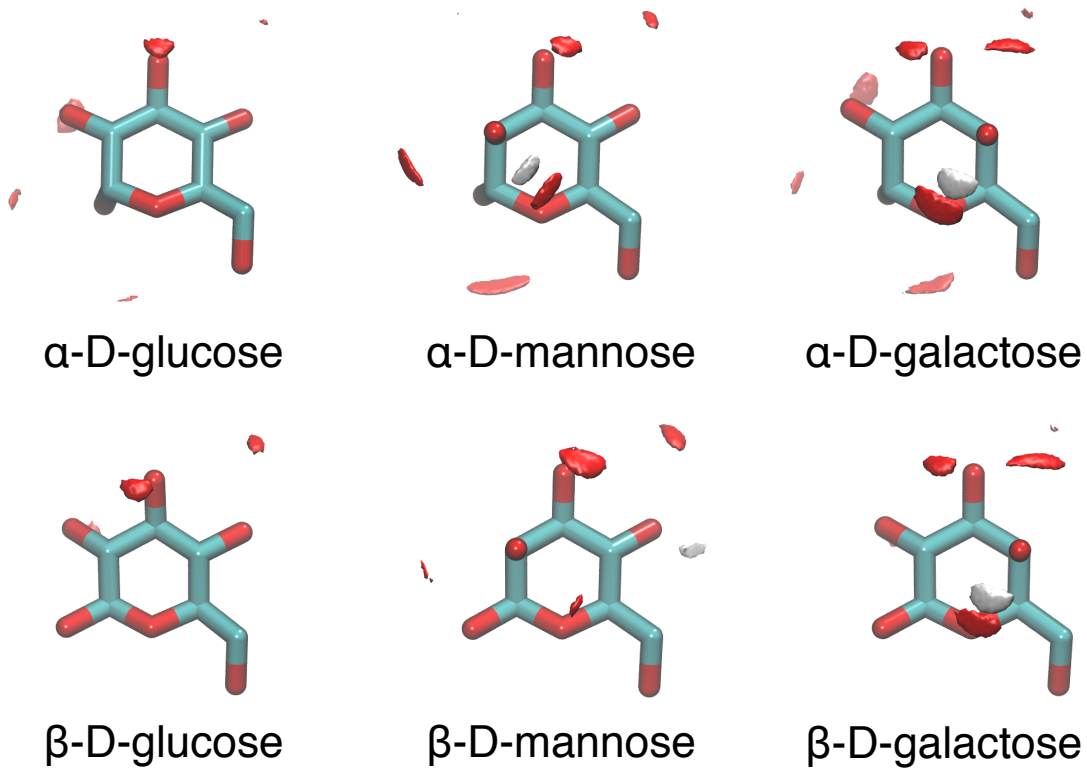


Figure S2: **SDFs of water molecules around each monosaccharide.** Only higher-value regions (more than 8.5 and 7.5 for oxygen and hydrogen atoms, respectively) are shown. The field is approximated on a square mesh with 0.1 Å mesh resolution.

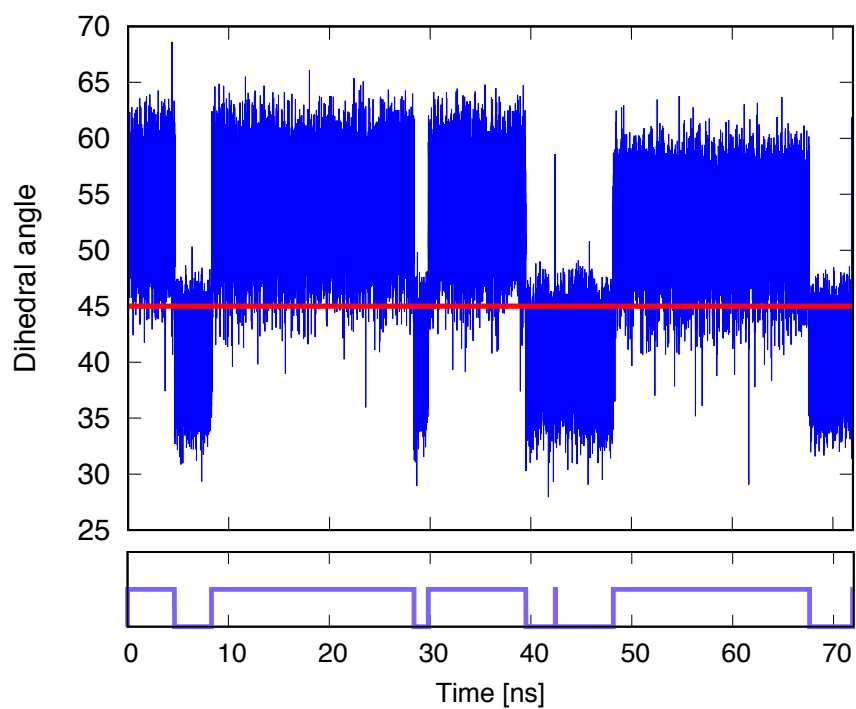


Figure S3: **Definition of the boat conformer.** Upper shows dihedral angle of a monosaccharide as a function of time with the threshold 45° . Lower shows the boat states during the simulation. The results show that our definition clearly separated two monosaccharide conformers.

Table S1: Average lifetime, content, and free energy change of the conformers in α -D-glucose.

| Temperature [K] | Concentration [M] | Lifetime [ns] | Content [%] | ΔG [kcal/mol] |
|-----------------|-------------------|---------------|-------------|-----------------------|
| 298 | 0.1 | 3.31 | 6.61 | 0.681 |
| 298 | 0.5 | 3.46 | 6.29 | 0.694 |
| 298 | 1.0 | 3.69 | 5.99 | 0.708 |
| 310 | 1.0 | 2.58 | 7.58 | 0.669 |
| 320 | 1.0 | 2.15 | 8.64 | 0.651 |
| 330 | 1.0 | 1.54 | 9.23 | 0.651 |
| 340 | 1.0 | 1.02 | 9.80 | 0.651 |
| 350 | 1.0 | 0.96 | 10.9 | 0.634 |

Table S2: Average lifetime, content, and free energy change of the conformers in α -D-mannose.

| Temperature [K] | Concentration [M] | Lifetime [ns] | Content [%] | ΔG [kcal/mol] |
|-----------------|-------------------|---------------|-------------|-----------------------|
| 298 | 0.1 | 0.56 | 4.10 | 0.810 |
| 298 | 0.5 | 0.67 | 4.26 | 0.800 |
| 298 | 1.0 | 0.63 | 4.06 | 0.813 |
| 310 | 1.0 | 0.40 | 4.71 | 0.804 |
| 320 | 1.0 | 0.38 | 5.30 | 0.796 |
| 330 | 1.0 | 0.30 | 5.96 | 0.785 |
| 340 | 1.0 | 0.25 | 6.32 | 0.791 |
| 350 | 1.0 | 0.20 | 6.59 | 0.801 |

Table S3: Average lifetime, content, and free energy change of the conformers in α -D-galactose.

| Temperature [K] | Concentration [M] | Lifetime [ns] | Content [%] | ΔG [kcal/mol] |
|-----------------|-------------------|---------------|-------------|-----------------------|
| 298 | 0.1 | 9.14 | 6.09 | 0.703 |
| 298 | 0.5 | 1.06 | 0.71 | 1.27 |
| 298 | 1.0 | 6.60 | 4.18 | 0.805 |
| 310 | 1.0 | 4.99 | 6.41 | 0.717 |
| 320 | 1.0 | 3.67 | 7.15 | 0.708 |
| 330 | 1.0 | 2.72 | 8.04 | 0.694 |
| 340 | 1.0 | 2.04 | 9.00 | 0.679 |
| 350 | 1.0 | 1.59 | 9.43 | 0.683 |

Table S4: Average lifetime, content, and free energy change of the conformers in β -D-glucose.

| Temperature [K] | Concentration [M] | Lifetime [ns] | Content [%] | ΔG [kcal/mol] |
|-----------------|-------------------|---------------|-------------|-----------------------|
| 298 | 0.1 | 0.24 | 0.28 | 1.51 |
| 298 | 0.5 | 0.28 | 0.36 | 1.45 |
| 298 | 1.0 | 0.22 | 0.25 | 1.54 |
| 310 | 1.0 | 0.18 | 0.38 | 1.50 |
| 320 | 1.0 | 0.15 | 0.48 | 1.47 |
| 330 | 1.0 | 0.12 | 0.57 | 1.47 |
| 340 | 1.0 | 0.10 | 0.69 | 1.46 |
| 350 | 1.0 | 0.07 | 0.79 | 1.46 |

Table S5: Average lifetime, content, and free energy change of the conformers in β -D-mannose.

| Temperature [K] | Concentration [M] | Lifetime [ns] | Content [%] | ΔG [kcal/mol] |
|-----------------|-------------------|---------------|-------------|-----------------------|
| 298 | 0.1 | 0.02 | < 0.00 | 2.58 |
| 298 | 0.5 | 0.01 | < 0.00 | 2.37 |
| 298 | 1.0 | 0.01 | < 0.00 | 2.40 |
| 310 | 1.0 | 0.01 | 0.01 | 2.46 |
| 320 | 1.0 | 0.01 | 0.02 | 2.35 |
| 330 | 1.0 | 0.01 | 0.03 | 2.31 |
| 340 | 1.0 | 0.01 | 0.03 | 2.38 |
| 350 | 1.0 | 0.01 | 0.04 | 2.36 |

Table S6: Average lifetime, content, and free energy change of the conformers in β -D-galactose.

| Temperature [K] | Concentration [M] | Lifetime [ns] | Content [%] | ΔG [kcal/mol] |
|-----------------|-------------------|---------------|-------------|-----------------------|
| 298 | 0.1 | - | - | - |
| 298 | 0.5 | 0.02 | < 0.00 | 2.75 |
| 298 | 1.0 | 0.19 | 0.03 | 2.09 |
| 310 | 1.0 | 0.02 | 0.01 | 2.46 |
| 320 | 1.0 | 0.02 | 0.01 | 2.54 |
| 330 | 1.0 | 0.11 | 0.05 | 2.16 |
| 340 | 1.0 | 0.18 | 0.14 | 1.93 |
| 350 | 1.0 | 0.13 | 0.17 | 1.92 |