Water structure modification by D-(+)-glucose at different concentrations and temperatures- effect of mutarotation

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Electronic supplementary information (ESI)

Fig. S1 Variation of change in free energy of activation for viscous flow, ΔG with the change in temperature from 0.5 M to 3.0 M concentration and in the temperature range of 20 ℃ to 60 ℃ temperature with the interval of 5 ℃.

Fig. S2 Variation of change in entropy of activation for viscous flow, ΔS with the change in (a) concentration of D (+)-glucose and (b) temperature. The concentration range was from 0.5 M to 3.0 M at the interval of 0.5 M and the temperature range was from 20 ℃ to 60 ℃ at the interval of 5 ℃.

Fig. S3 Variation of the activation enthalpy change for viscous flow with the variation of (a) concentration of D (+)-glucose and (b) temperature. The concentration range was from 0.5 M to 3.0 M at the interval of 0.5 M and the temperature range was from 20 ℃ to 60 ℃ at the interval of 5 ℃.

Fig. S4 Size distribution of aggregates formed in (a) 1.5 M, (b) 2.0 M, (c) 2.5 M, and (d) 3.0 M aqueous solution of D-(+)-glucose. The size, i.e., hydrodynamic diameter (nm) of the aggregates formed in each temperature is stacked in each layer from 20 ℃ to 60 ℃. The X-axis is plotted in logarithmic scale and the Y-axis of each layer is plotted in linear scale from 0 to 100% of intensity.

Fig. S5 Size distribution of aggregates formed in different concentrations of D (+)-glucose aqueous solutions. The size, i.e., hydrodynamic diameter (nm) of the aggregates formed in each concentration is stacked in each layer from 0.5 M to 3.0 M. The X-axis is plotted in logarithmic scale and the Y-axis of each layer is plotted in linear scale from 0 to 100% of intensity.

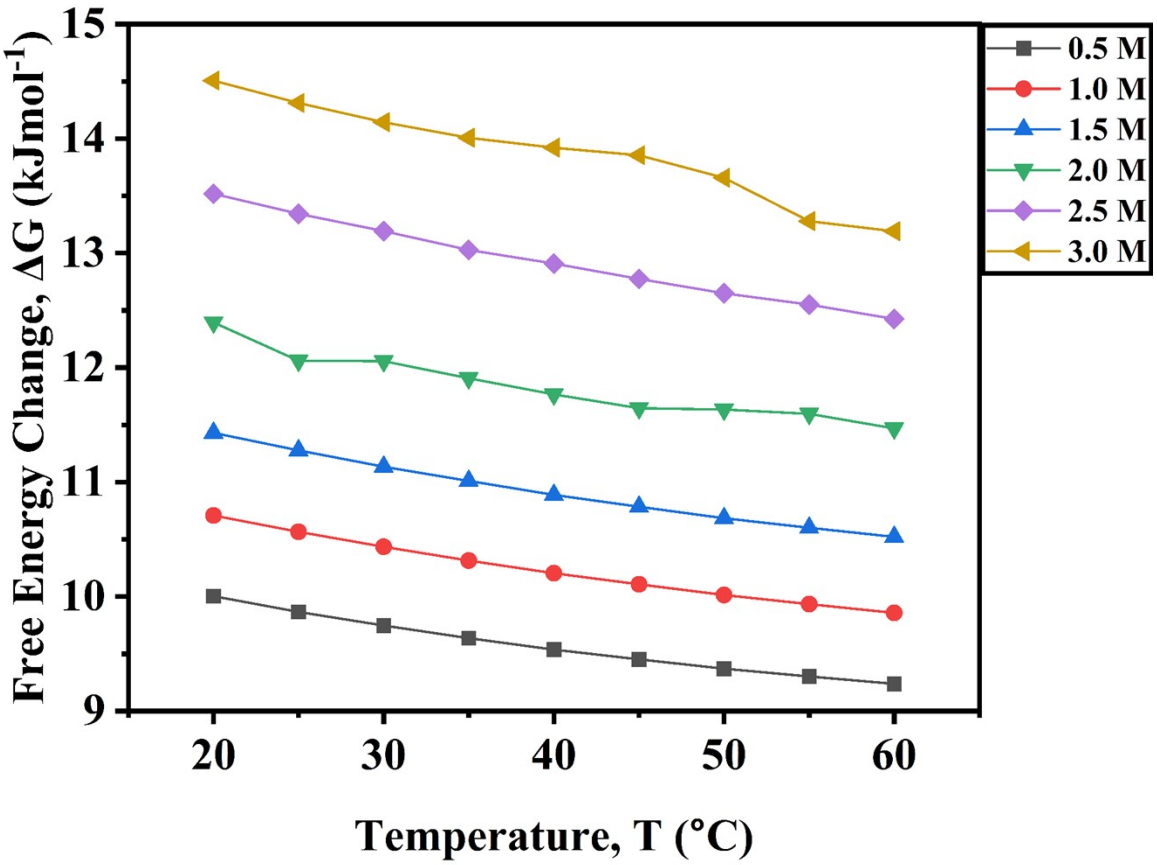
Fig. S6 Difference spectra of aqueous α-D-glucose solutions at 1.00 M, 1.50 M, 2.00 M, and 2.50 M concentrations measured after 12 min, 18 min, 24 min, and 30 min with reference to the first spectrum measured at 6 min. Range in the X-axis is from 4400 cm^{-1} to 5800 cm^{-1} and the range in the Y-axis is from -0.0025 to 0.0025 for each plot.

Fig. S7 Difference spectra of aqueous α-D-glucose (top) and β-D-glucose (bottom) solutions of 0.25 M concentration at 30 ℃ (left) and 55 ℃ (right) at 24 min and 30 min with reference to the first spectrum measured at 12 min.

Fig. S8 Change of band positions of hydrogen-bonded components of aqueous α-D-glucose (top) and β-D-glucose (bottom) solutions with temperature. The positions of these bands are constant with increasing temperature.

Fig. S9 Time-dependent synchronous 2D NIR correlation spectra of 2.5 M aqueous α-D-glucose (top) and β-D-glucose (bottom) solutions. The positive peaks are colored red and the negative peaks are colored blue. The two autopeaks along the diagonal are disproportionate to each other and the sign of the cross-peaks are both negative.

Fig. S10 Refractive indices of α-D-glucose and β-D-glucose solutions of 2.50 M concentration at different time intervals up to 30 min.



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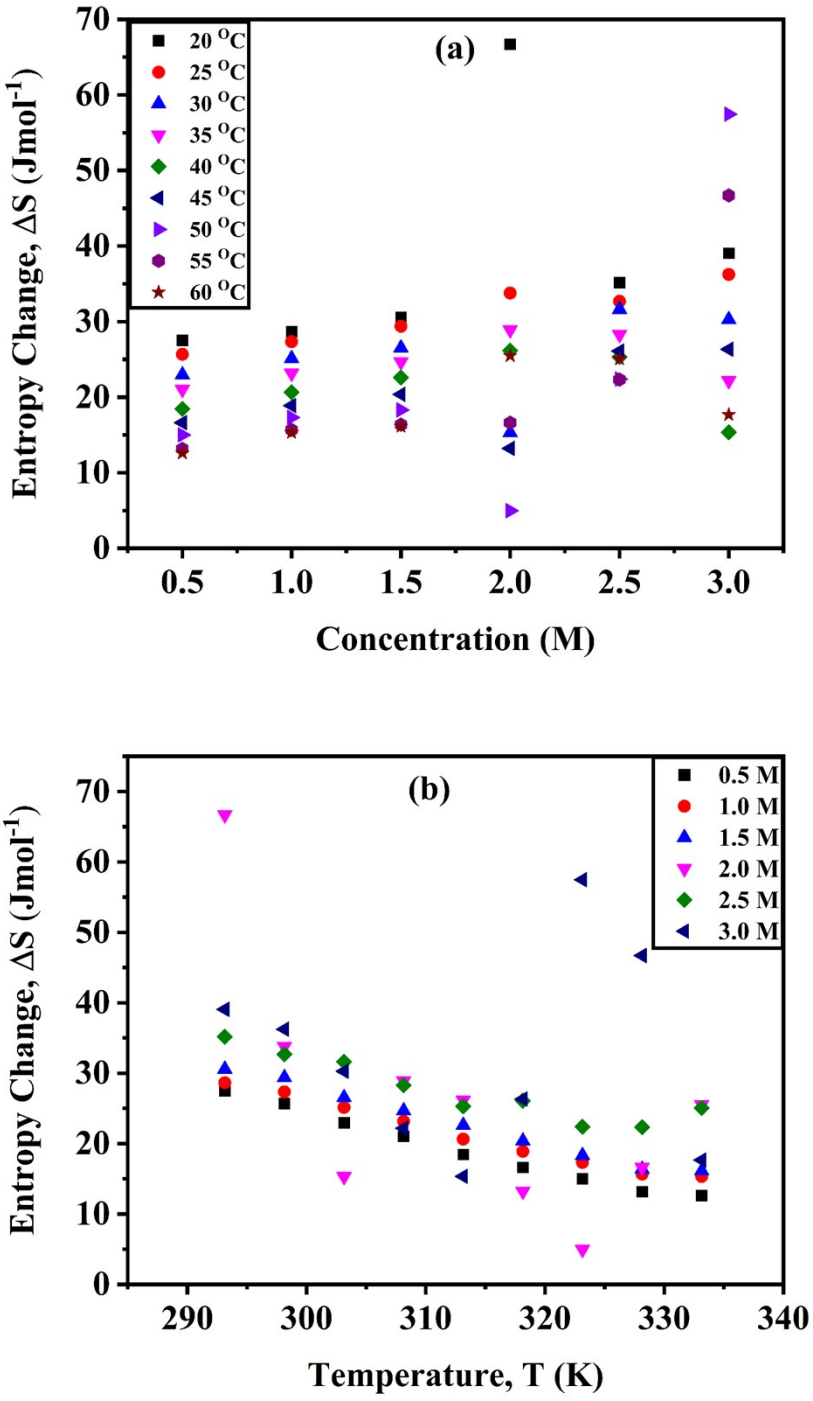
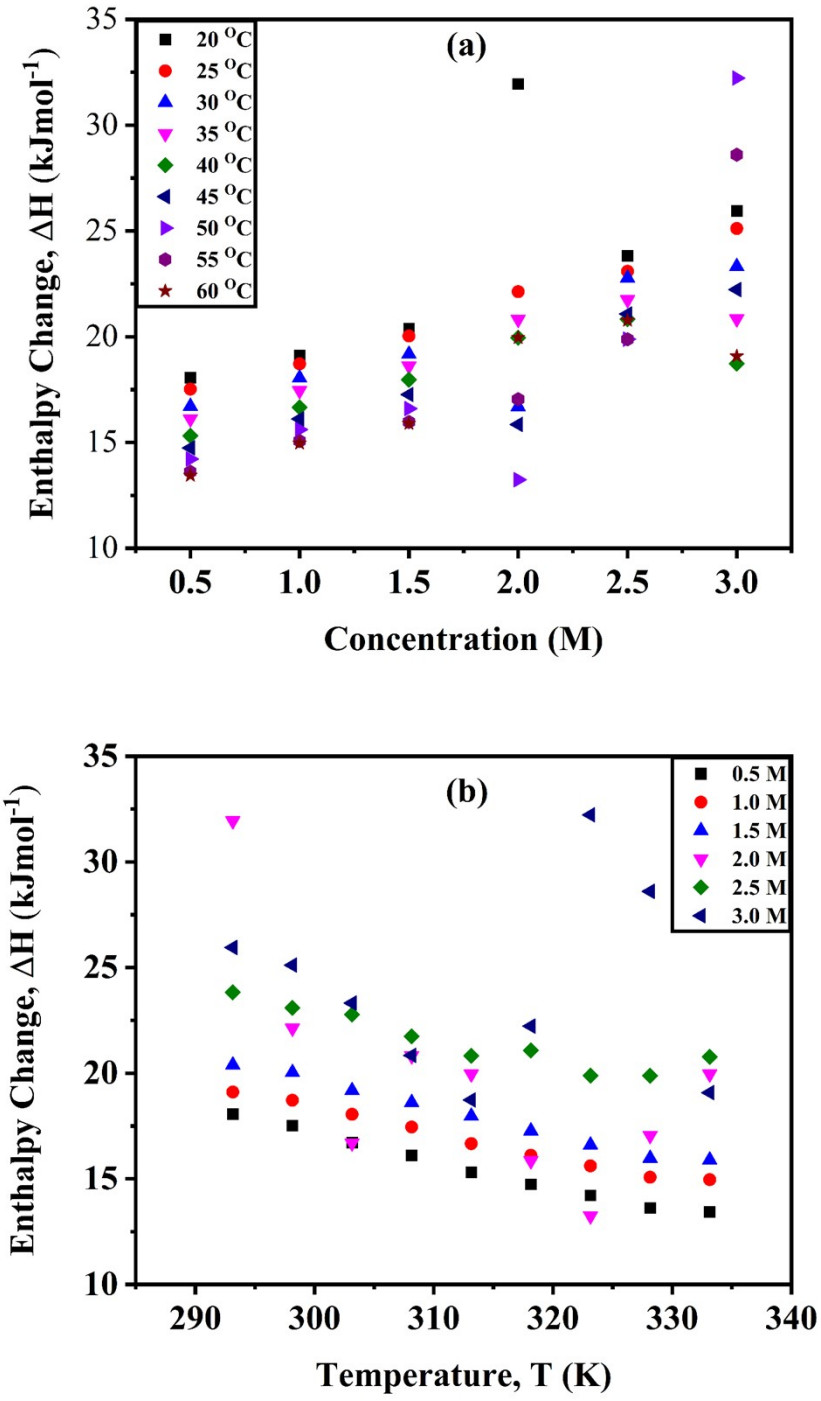


Fig. S2 Variation of change in entropy of activation for viscous flow, Δ*S* with the change in (a) concentration of D (+)-glucose and (b) temperature. The concentration range was from 0.5 M to 3.0 M at the interval of 0.5 M and the temperature range was from 20 ℃ to 60 ℃ at the interval of 5 ℃.



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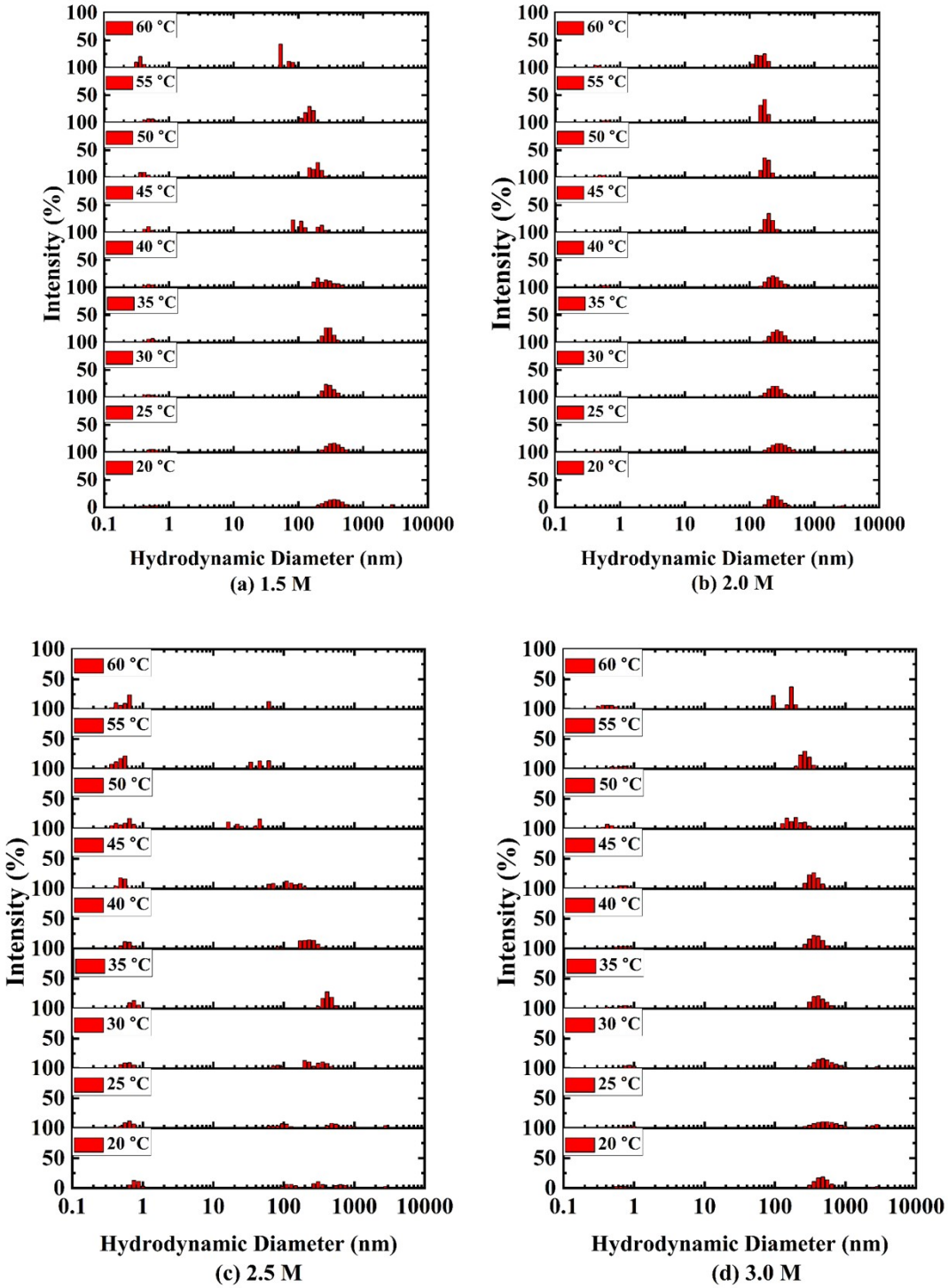

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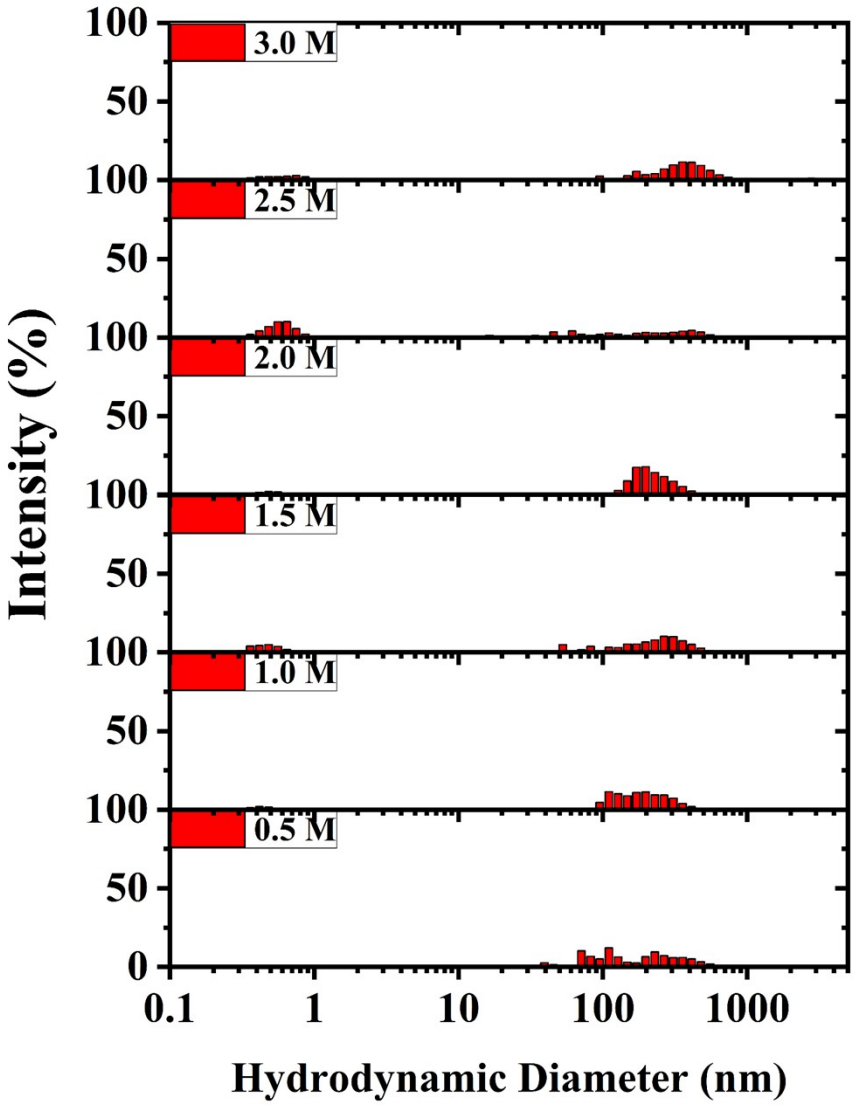

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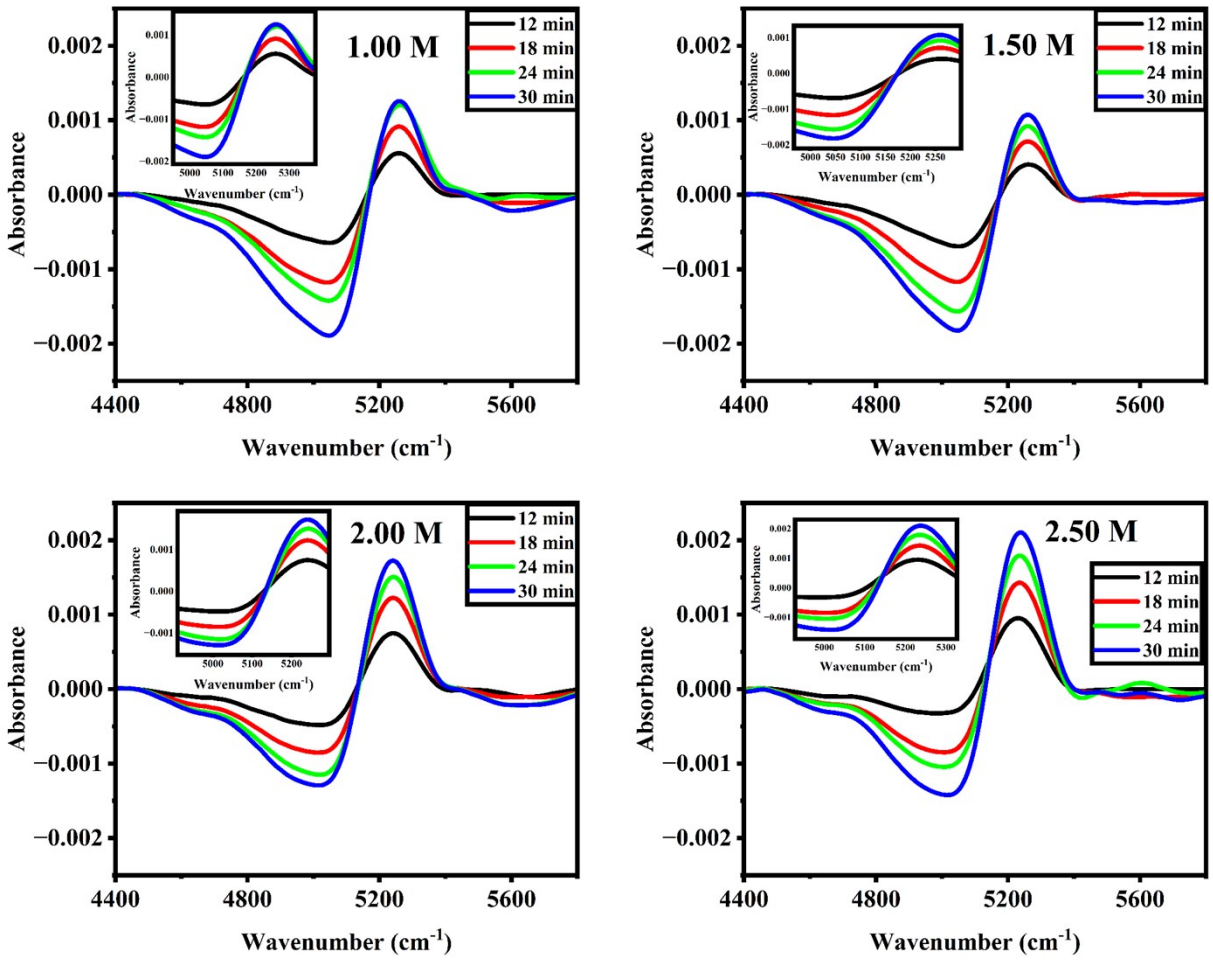

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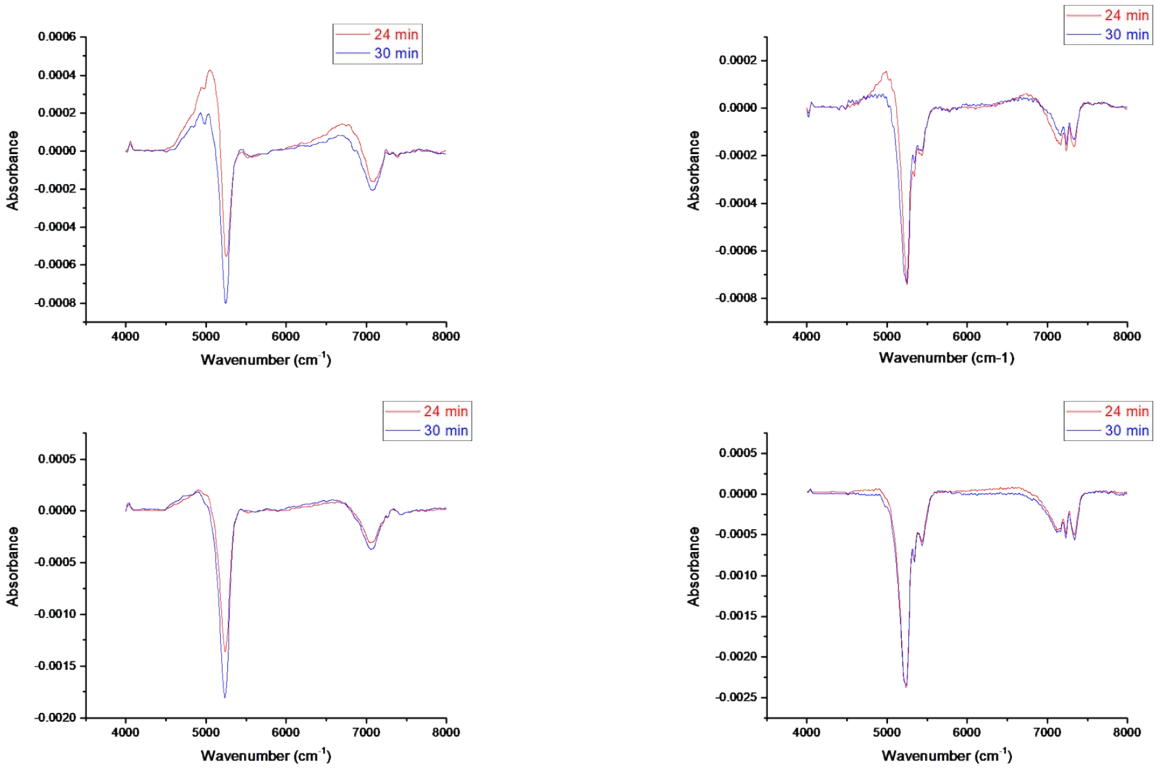

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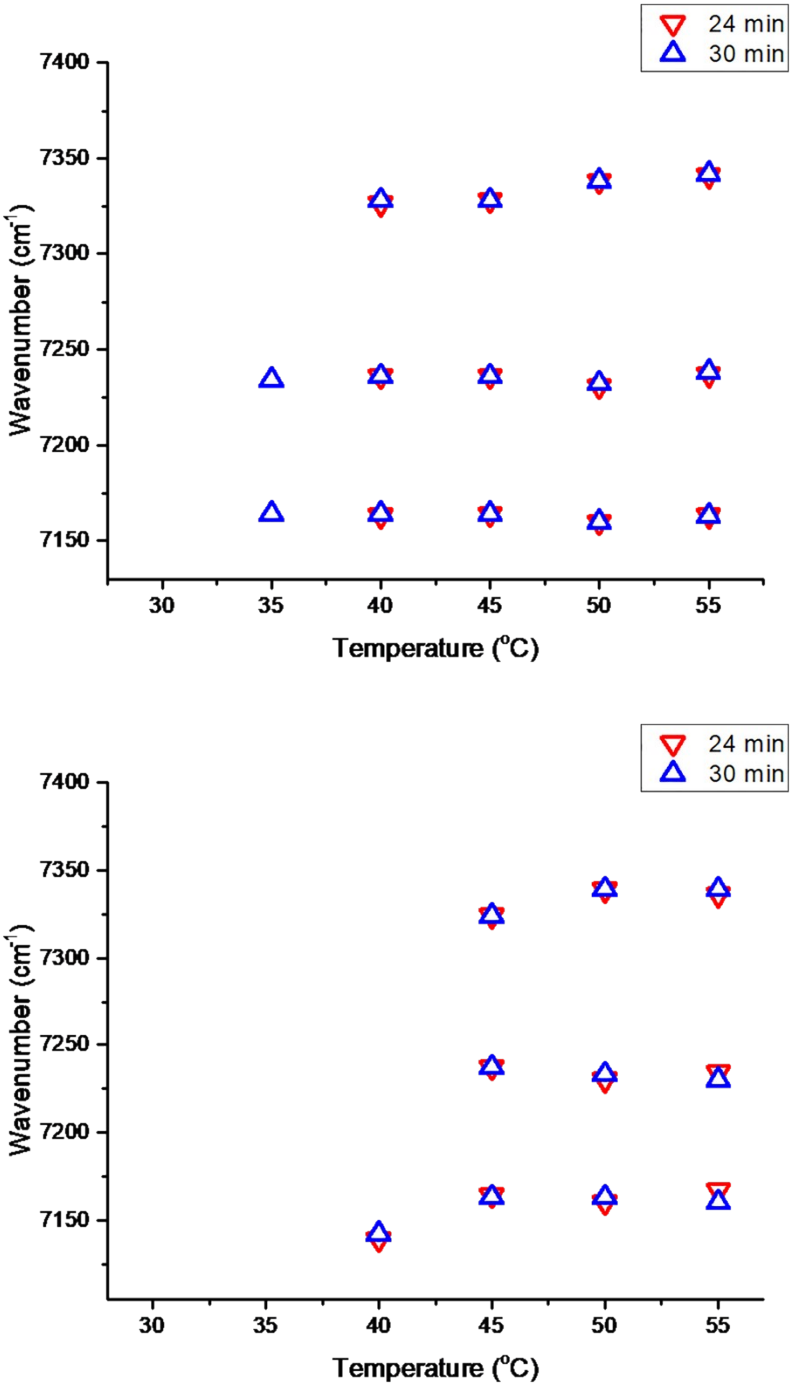

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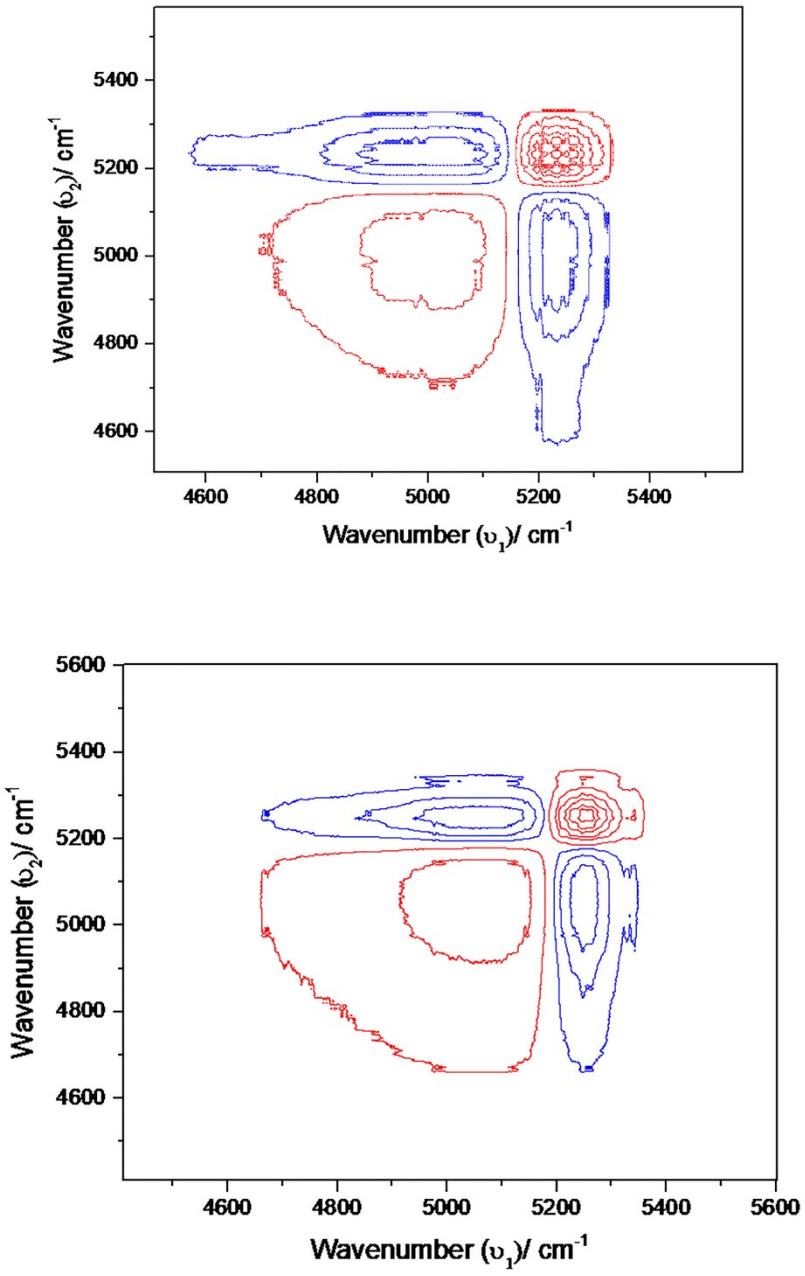

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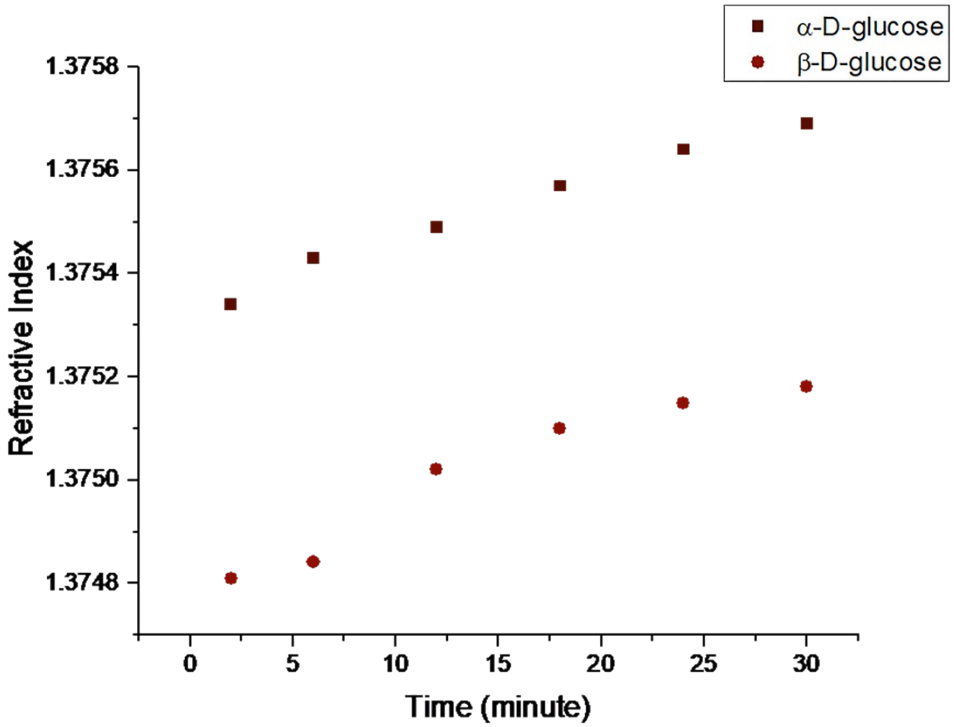

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