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**Supporting information for article:**

# Thermal contraction of aqueous glycerol and ethylene glycol solutions for optimized protein crystal cryoprotection

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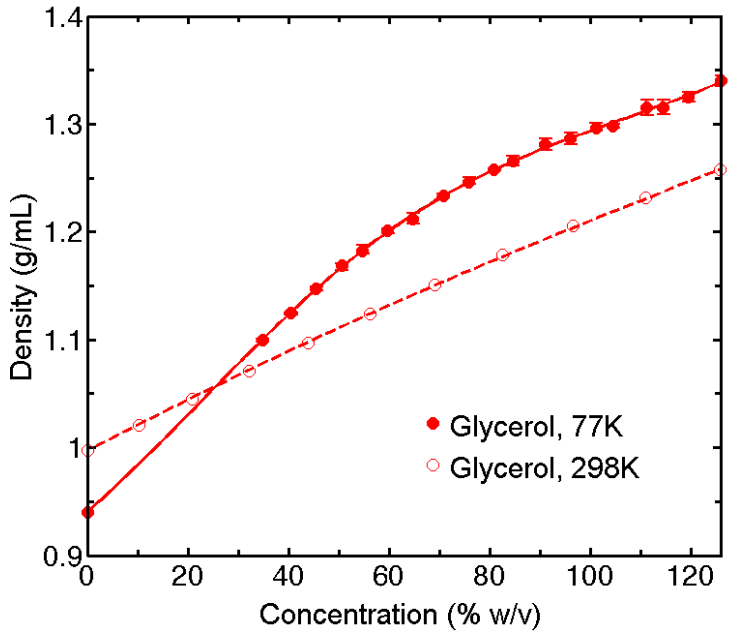
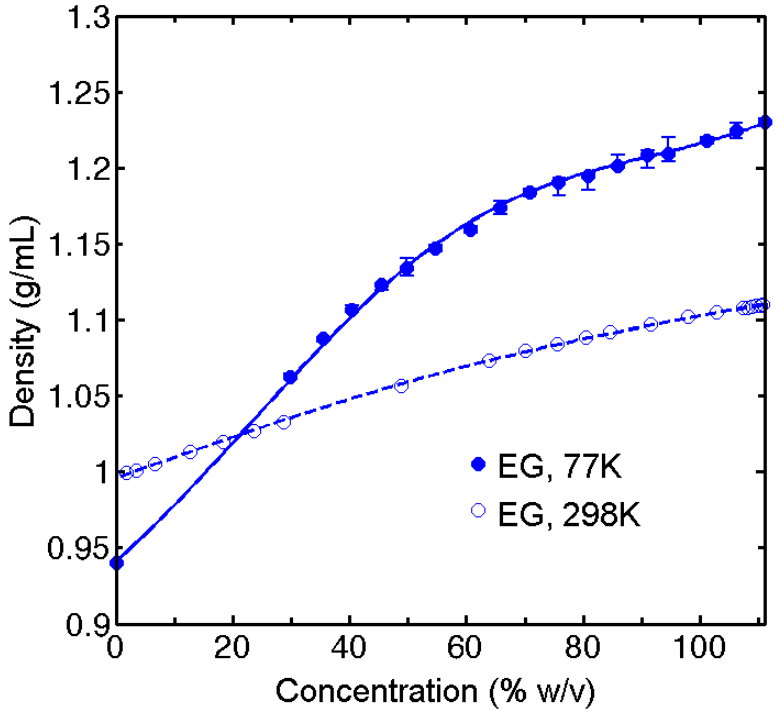
**Table S1** Parameters for the fits to the excess specific volume in Figure 3 and S2 given by Equation 8, obtained by nonlinear regression, and for fits to the density in Figure 2 given by Equation 9.

| Parameter | Glycerol | | Ethylene Glycol | |
|---|---|---|---|---|
| | 298 K | 77 K | 298 K | 77 K |
| $a_0$ | -0.0164 | -0.118 | -0.0236 | -0.114 |
| $a_1$ | 53.01 | 49.39 | 52.89 | 49.14 |
| $a_2$ | 40.18 | 39.49 | 44.28 | 37.91 |
| $a_3$ | 0.00695 | 0.0541 | 0.0127 | 0.0489 |

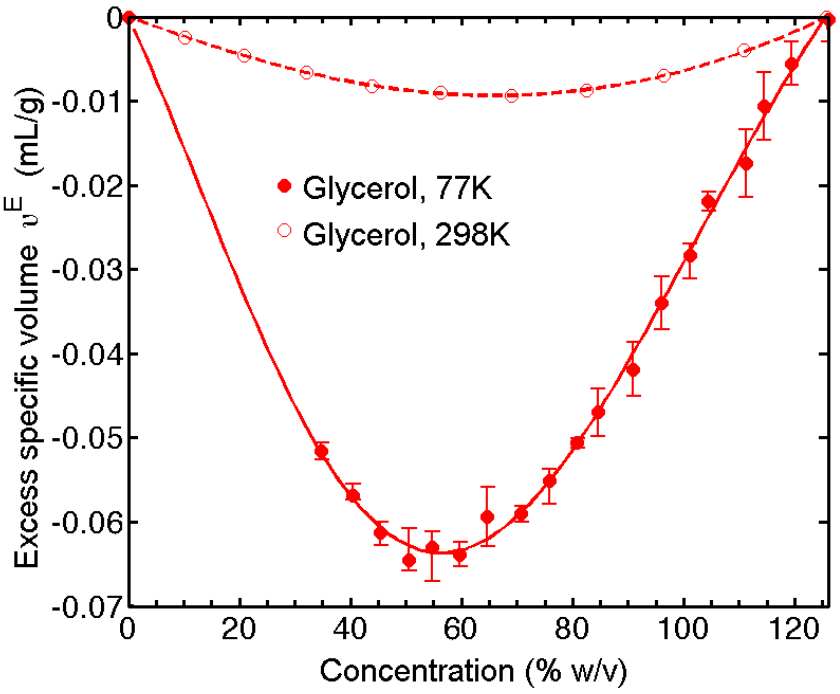



**(a)**

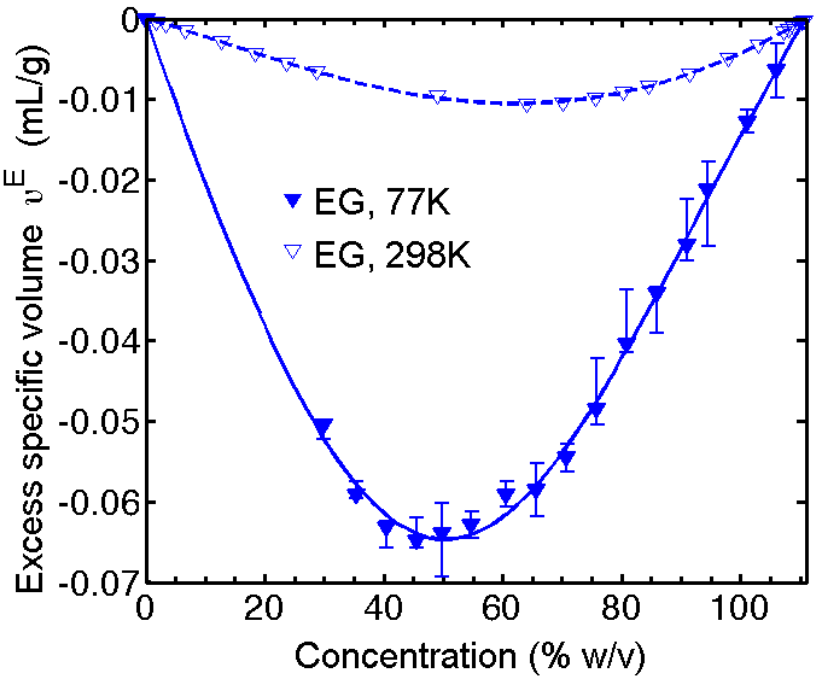



**(b)**

**Figure S1** Measured density versus cryoprotectant concentration in % (w/v) at 77 K and literature values (Bosart & Snoddy, 1928; Rodrigues & Francesconi, 2011) at 298 K for (a) glycerol and (b) ethylene glycol. The solid and dashed lines are fits given by Equations 8 and 9, and with parameters as given in Table **S1**.




(a)




(b)

**Figure S2** Excess specific volume $V^E = V_{actual} - V_{ideal}$ versus cryoprotectant concentration in % (w/v) at 77 K and 298 K for (a) glycerol and (b) ethylene glycol, calculated using Equations 5 and 6 and the densities in Figure 2. The solid lines are fits given by Eq. 8, with parameters as given in Table **S1**.

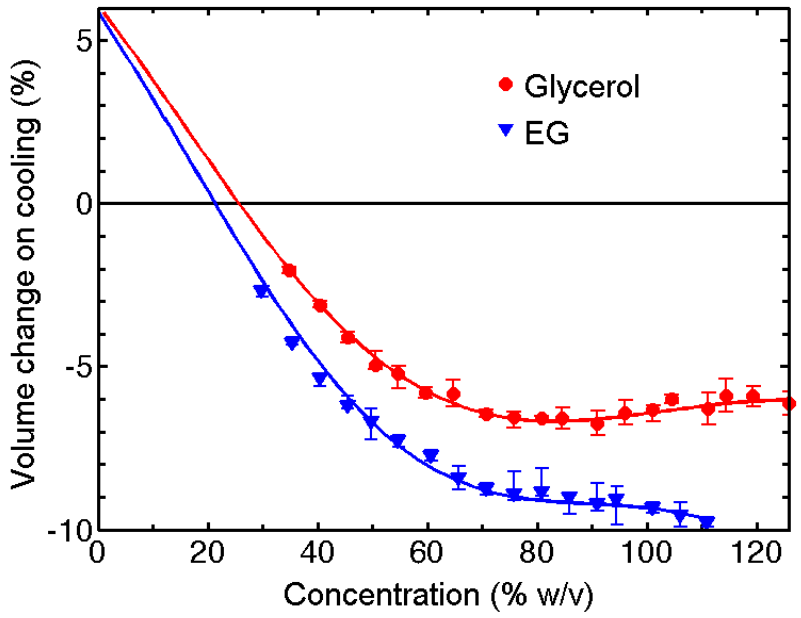



**Figure S3** Change in density between 298 K and 77 K vs. cryoprotectant concentration in % (w/v) for aqueous glycerol and ethylene glycol solutions. Data points are given by the difference between data points at 77 K and a fit to the measured (and more accurate) 298 K values. Fits are given by the difference between the fits to the 77 K and 298 K data in Figure 2.

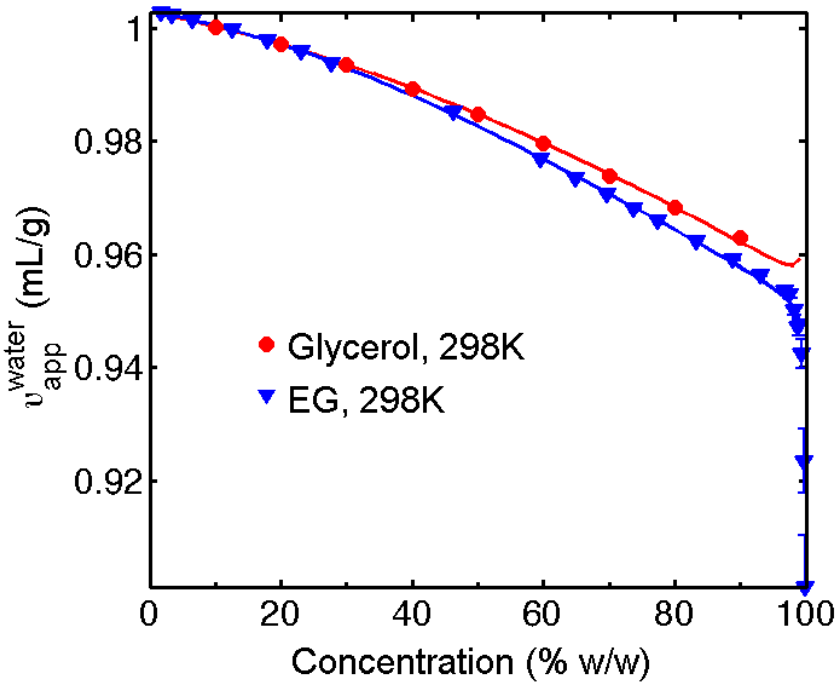



**Figure S4** Apparent specific volumes of water calculated using Equation 11 vs. cryoprotectant concentration in % (w/w) for ethylene glycol and glycerol in water at 298 K.