

A. G. Filoteo, N. Juranic, A. Penheiter, A. J. Caride, J. T. Penniston, and E. E. Strehler. 2007. The C-terminal tail of human plasma membrane calcium ATPase isoform 4b is intrinsically disordered. *Biophys. J.* (Suppl. S):8A (Abstr.)

The list of authors should have included Dr. Sergei Venyaminov, who did the work on circular dichroism measurements and analyses for this study. The authorship should have appeared as written below:

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Cristina S. Pereira, David Kony, Riccardo Baron, Martin Müller, Wilfred F. van Gunsteren, and Philippe H. Hünenberger. 2006. Conformational and dynamical properties of disaccharides in water: a molecular dynamics study. *Biophys. J.* 90:4337–4344.

We recently reported a detailed analysis of the conformational and dynamical properties of the eight reducing glucose disaccharides based on explicit-solvent molecular dynamics simulations with the GROMOS 45A4 force field. Unfortunately, due to an error in the reconstruction of the molecular connectivity by application of periodic boundary conditions along the trajectories, the reported results for the analysis of the configurational entropies (Fig. 3 and Table 4 of the original article) were incorrect. The problem only occurred for this specific analysis, and did not affect all other reported analyses (distribution of glycosidic dihedral angles, occurrence of intramolecular hydrogen bonds, and dynamics of the dihedral angles).

The corrected results are reported in Table 1 and Fig. 1 of this erratum, replacing Table 4 and Fig. 3 of the original article, for the disaccharides kojibiose (**K**), sophorose (**S**), nigerose (**N**), laminarabiose (**L**), maltose (**M**), cellobiose (**C**), isomaltose (**I**), and gentiobiose (**G**). Fig. 1 displays, for each disaccharide, the cumulative configurational quasi-harmonic entropy estimate

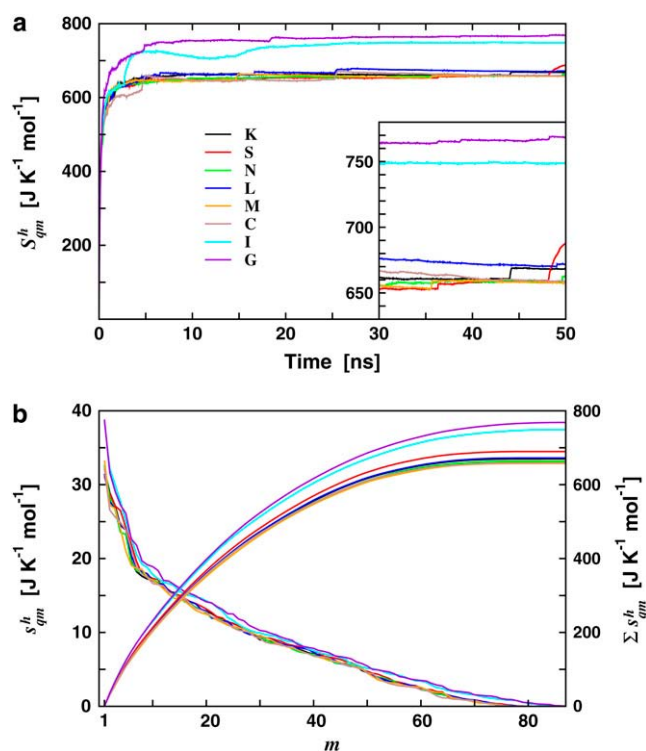


FIGURE 1 Buildup curves of the quasi-harmonic entropy S_{qm}^h for the eight disaccharides considered as a function of the sampling time (*a*; the *inset* focuses on the last 20 ns of the main panel), and corresponding entropy contributions $s_{qm}^h(m)$ per mode (based on the full 50 ns simulations) displayed as a function of the eigenvector index m (*b*; *left scale and decreasing curves*) together with the corresponding cumulative sum (*b*; *right scale and increasing curves*).

TABLE 1 Estimated configurational entropies and corresponding correction terms for the eight disaccharides considered

| Sugar | S_{qm}^{h} [$J \times K^{-1} \times \text{mol}^{-1}$] | $\Delta S_{\text{cl}}^{\text{ah}}$ [$J \times K^{-1} \times \text{mol}^{-1}$] | $\Delta S_{\text{cl}}^{\text{pc}}$ [$J \times K^{-1} \times \text{mol}^{-1}$] | S^{ctd} [$J \times K^{-1} \times \text{mol}^{-1}$] | $-T\Delta S^{\text{ctd}}$ [$kJ \times \text{mol}^{-1}$] |
|----------|--|--|--|--|--|
| K | 669 | −1 | −13 | 655 | −6.85 |
| S | 688 | −2 | −17 | 669 | −11.03 |
| N | 663 | −2 | −15 | 646 | −4.17 |
| L | 671 | −1 | −18 | 652 | −5.96 |
| M | 657 | −2 | −16 | 639 | −2.09 |
| C | 658 | −3 | −23 | 632 | 0.00 |
| I | 749 | −2 | −9 | 738 | −31.60 |
| G | 769 | −2 | −14 | 753 | −36.08 |

S_{qm}^{h} as a function of the sampling time (*top*) and the corresponding contribution s_{qm}^{h} per mode as a function of the eigenvector index m , together with its cumulative sum (*bottom*; for the 50 ns simulations). Table 1 reports, for each disaccharide, the quasi-harmonic entropy estimate S_{qm}^{h} (for the 50 ns simulations and including contributions from all quasi-harmonic modes), and the associated corrections $\Delta S_{\text{cl}}^{\text{ah}}$ for anharmonicity in the individual modes and $\Delta S_{\text{cl}}^{\text{pc}}$ for (supralinear) pairwise correlations among the different modes, and the corrected value $S^{\text{ctd}} = S_{\text{qm}}^{\text{h}} + \Delta S_{\text{cl}}^{\text{ah}} + \Delta S_{\text{cl}}^{\text{pc}}$.

Although the calculated entropies S^{ctd} are significantly lower than initially reported, and the detailed ranking of the disaccharides in terms of decreasing entropies is slightly altered (**G** > **I** >> **S** > **K** > **L** > **N** > **M** > **C** as opposed to **G** >> **I** >> **L** > **S** > **K** > **N** > **M** >> **C** initially reported), the main conclusions of the study concerning entropy are not affected. We still observe: 1), a significantly higher entropy for (1 → 6)-linked disaccharides (**I** and **G**); 2), a significantly lower entropy for **C** compared to all disaccharides investigated; and 3), a higher entropy for the β -form compared to the α -form of a given linkage (except for the **M/C** pair).