

ADDITIONS AND CORRECTIONS

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Markus Christen, Anna-Pitschna E. Kunz, and Wilfred F. van Gunsteren*: Sampling of Rare Events Using Hidden Restraints

Pages 8488–8498. To our dismay we have found an error in the calculations reported in the paper in ref 1.

A new method to calculate the free energy difference between different conformations of β -D-glucopyranoside implemented by Hansen and Hünenberger found significantly different results to the ones we reported in ref 1. This led to a rechecking of the simulation code where an error in the implementation of eqs (18) and (19) (on p 8490 of ref 1) was found and corrected by Oostenbrink.

The application section “Conformations of a Cyclic Aminoxy-Hexapeptide upon Binding Cations and Anions” was unaffected by these changes.

The calculations for the section “Relative Stabilities of Hexopyranose in 4C_1 vs 1C_4 Conformation” were repeated. The simulation parameters were the same as described in ref 1 except that more λ -values were simulated (41 instead of 11 equally distributed discrete λ points between 0 and 1) and at each λ -value the system was simulated for a longer time (200 ps of equilibration instead of 50 ps followed by 4 ns of simulation instead of 150 ps) with a much stronger force constant $K^{\text{dih}} = 1000 \text{ kJ/rad}^2$ instead of 10 kJ/rad^2 .

The free energy difference between the two conformations is now calculated to be $14.7 \pm 1.4 \text{ kJ/mol}$ for the change 4C_1 to 1C_4 and $-15.0 \pm 1.5 \text{ kJ/mol}$ backward. The values reported in ref 1 on page 8493 were $4.6 \pm 3.4 \text{ kJ/mol}$ for 4C_1 to 1C_4 and $-5.6 \pm 2.5 \text{ kJ/mol}$ backward. The new results are still compatible with the integrated potential of mean force which claims a relative free energy difference between the 4C_1 and the 1C_4 state of $8.6 \pm 10.2 \text{ kJ/mol}$ (ref 1 p 8494). Only minor changes could be seen in Figure 7 on page 8493 (not shown). The differences in Figure 8 on page 8493 were more distinct. A comparison between the old and the new curves are shown in Figure 1. The new results are now in agreement with the ones to be reported by Hansen and Hünenberger.

The conclusions drawn from the results remain unchanged. The authors would like to apologize for the inconvenience to the reader.

References and Notes

- (1) Christen, M.; Kunz, A.-P. E.; van Gunsteren, W. F. *J. Phys. Chem. B* **2006**, *110*, 8488.

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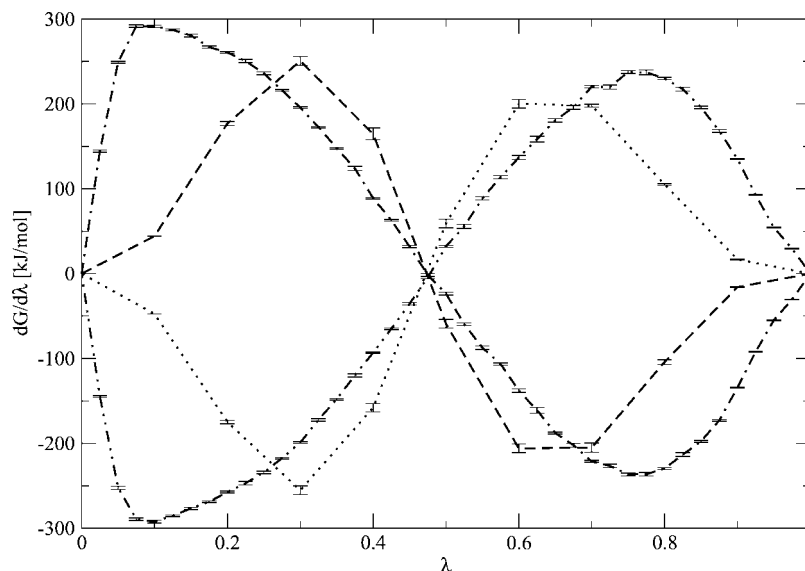


Figure 1. Average derivative of the Hamiltonian with respect to the pathway coordinate λ during a multiconfigurational thermodynamic integration of β -D-glucopyranoside. The dashed line corresponds to a conformational change from 4C_1 ($\lambda = 0$) to 1C_4 ($\lambda = 1$) for the old (erroneous) simulation, the dash-dash-dotted line for the new simulation. The dotted line represents the reverse isomerization for the old (erroneous) simulation, the dash-dot-dotted for the new one.