



CORRECTION

## Correction to: Conformational analysis of xylobiose by DFT quantum mechanics

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### Correction to:

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During the preparation of a follow-on manuscript, it was discovered that values of the temperatures of the distribution were miscalculated. The correct formula for the temperature is  $T = 1/(\text{coefficient} \cdot R)$ , where  $R = 0.001987$  (the universal gas constant in kcal/(deg mol) and coefficient is the parameter from the exponential curve fitting  $y = e^{-\text{coefficient} \cdot x}$  where  $y$  is the probability of structures with each energy value, and  $x$  is the value of the energy.

In Table 2, the correct values for the first column of Temperatures

|  |                                       |
|--|---------------------------------------|
| Solvated xylobiose, QM                     | <del>529</del> Correct<br>value = 479 |
| Solvated THP-O-THP, QM                     | <del>662</del> Correct<br>value = 382 |
| Martínez-Abad et al. (2017) Glycam<br>POMF | <del>542</del> Correct<br>value = 468 |

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