

## Comment on the calculations in protein thermodynamics

DOI 10.1074/jbc.L118.002358

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Edited by Luke O'Neill

We found a recent paper (1) that would be valuable in the field of protein thermodynamics. However, the paper contains some calculation errors. Here, we discuss the errors. Following the notations in Table 2 of the paper, the ensuing relationship of entropy can be established.

$$T\Delta S^0_{\text{Maltose: MBP}} + T\Delta S^0_{\text{MBP: sAB-11M in 1 mM maltose}} = T\Delta S^0_{\text{MBP: sAB-11M}} + T\Delta S^0_{\text{Maltose: MBP in 5-fold molar excess sAB-11M}}$$

Plugging the corresponding values reported in Table 2 of the paper to the equation does not satisfy the equality:  $10.4 + (-2.0) \neq 5.6 + 2.0$  (in kcal/mol).

Secondly, there are errors made in the calculation of  $\Delta G^0$  in Table 2. Based on the equation,  $\Delta G^0 = \Delta H^0 - T\Delta S^0$  (2), we found that  $\Delta G^0_{\text{MBP: sAB-11M in 1 mM maltose}} = -14 -$

$(-2) = -12$  kcal/mol, not  $-11.4$  kcal/mol as stated in the paper.  $\Delta G^0_{\text{Maltose: MBP in 5-molar excess of sAB-11M}} = -8.9 - 2 = -10.9$  kcal/mol, not  $-11.1$  kcal/mol.  $\Delta G^0_{\text{Maltose: MBP in 5-molar excess of sAB-P1}} = -14 - (-1.0) = -13$  kcal/mol, not  $-12.6$  kcal/mol.

The third error we found is with  $K_D$  for the binding of MBP to sAB-P1 in 1 mM maltose in Table 2:  $K_D = \exp(\Delta G^0/RT) = \exp(-11,000 \text{ cal/mol} \times 4.184 \text{ J/cal} / (8.314 \text{ J/mol K} \times 298.15 \text{ K})) = 8.6 \text{ nM}$ , not  $0.9 \text{ nM}$  as in the paper. Lastly,  $K_{\text{mal}}$  and  $K_{\text{sAB}}$  in Fig. 5 are  $0.83 \times 10^{-6} \text{ M}$  and  $0.47 \times 10^{-6} \text{ M}$ , not  $0.83 \times 10^{-3} \text{ M}$  and  $0.47 \times 10^{-3} \text{ M}$ , respectively.

### References

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The authors declare that they have no conflicts of interest with the contents of this article.

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