

Correction to Microscopic Analysis of Protein Oxidative Damage: Effect of Carbonylation on Structure, Dynamics, and Aggregability of Villin Headpiece

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Page 7020, Figure 5. The reported molecular hydrophobicity potential (MHP) values of the carbonylated residues amino-adipic semialdehyde (Asa) and glutamic semialdehyde (Gsa) were calculated using a different procedure than MHP values of canonical residues. Briefly, the former were calculated for amino acid side chain analogs, while the latter were calculated for complete amino acids with subsequent subtraction of the values for the backbone atoms. While both procedures are in principle sound, a direct comparison of the two sets mandates that a common procedure be used. The fully consistent, corrected values using the latter procedure are 0.62 and 0.16, for Asa and Gsa, respectively, rather than the originally reported 1.56 and 1.27. Importantly, this does not change any of the principal conclusions of the study, but does affect several of its quantitative aspects. Primarily, estimated changes in the aggregability of positively charged proteins upon carbonylation of lysine and arginine should be $\ln(v_{\text{mut}}/v_{\text{wt}}) = 2.47 \pm 0.73$, (Lys to Asa) and $\ln(v_{\text{mut}}/v_{\text{wt}}) = 2.78 \pm 0.73$ (Arg to Gsa), rather than 3.37 ± 0.73 and 3.85 ± 0.73 , respectively, and 1.49 ± 0.73 and 1.80 ± 0.73 , rather than 2.39 ± 0.73 and 2.87 ± 0.73 for negatively charged proteins. Additionally, in terms of MHP weights, converting Lys to Asa or Arg to Gsa is similar to mutating them to more hydrophobic methionine and threonine, respectively, rather than leucine and valine as originally reported. Accordingly, several statements in the original article should be modified as follows:

- (1) Page 7021. “The effect of carbonylating Pro to Gsa is less dramatic, albeit still resulting in a net increase in hydrophobicity...” should read “On the other hand, the effect of carbonylating Pro to Gsa results in a slight net decrease in hydrophobicity...”.
- (2) Page 7022. “... more than a 30- to 40-fold increase...” should read “... more than a 10- to 15-fold increase...”.

- (3) Page 7022. “... only 2 out of 27 such mutations having a greater effect...” should read “... only 3 (2 in the case of arginine carbonylation) out of 27 such mutations having a greater effect...”.
- (4) Page 7022. “... from an unfavorable -1 to a highly favorable 0.5 .” should read “...from an unfavorable -1 to a highly favorable 0.6 .”

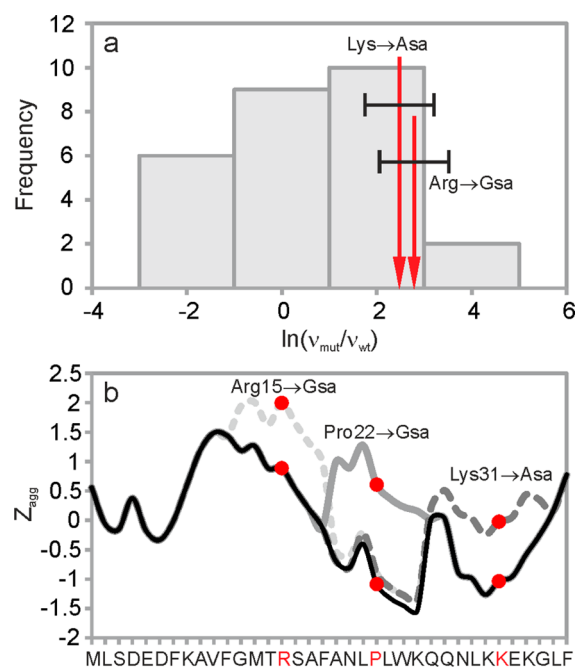


Figure 7.

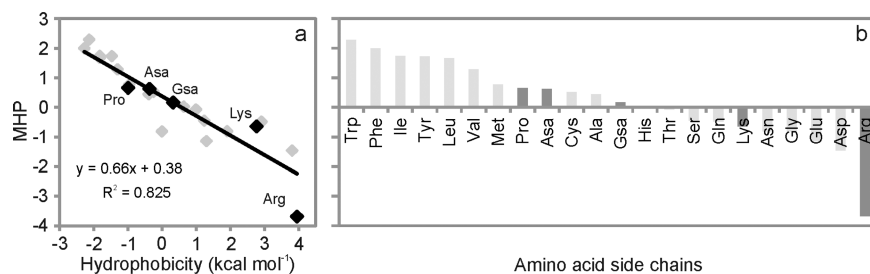


Figure 5.

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Corrected versions of graphics that are affected by this change (the table of contents graphic and Figures 5 and 7 are shown below. Supporting Information (SI) Figure S3 and Table S1 have also been updated in the corrected SI file.

